File Ref.No.Ac.A3/Faculty of Science/2023 (PART-I)

COCHIN UNIVERSITY OF SCIENCE AND TECHNOLOGY

(Abstract)

Faculty of Science - Revised course structure and syllabi of M.Sc. Chemistry Programme effective from 2024 admission onwards - Resolution of the Academic Council - Communicated - Orders issued.

ACADEMIC A SECTION

No.CUSAT/AC(A).A3/3584/2024 Dated,KOCHI-22,22.08.2024

Read:-Item No. I (g)(5) of the minutes of the meeting of the Academic Council held on 30.04.2024

ORDER

The Academic Council considered along with the recommendations of its standing committee, the Minutes of the Faculty of Science held on 08.04.2024 and resolved to approve the revised course structure and syllabus for M.Sc.Chemistry programme with effect from 2024 admissions (appended)

Orders are, therefore, issued accordingly.

Dr. V. Sivanandan Achari *
Registrar

To:

1. The Dean, Faculty of Science
2. Chairmen, BoS under Faculty of Science
3. The Head, Department of Applied Chemistry
4. All AR/DR Examination wing - with a request to forward to concerned sections
5. The Director,IQAC/ DoA
6. CIRM/Conference Sections
7. PS To VC/PVC;PA To Registrar/CE.

* This is a computer generated document. Hence no signature is required.

Appendix -1

Department of Applied Chemistry

Cochin University of Science and Technology

M.Sc. Chemistry Syllabus

2024-25

Programme Objective

The M. Sc. course in Chemistry aims to build human resources in the area of Chemical Science and create trained competent manpower which can take up any challenges in teaching and research.

Programme Specific Outcomes

On successful completion of M. Sc. Chemistry programme, students will possess

PSO 1: Systematic and coherent awareness in fundamentals and its applications in problem solving, and analytical and critical rationalizations.

PSO 2: A firm grip on the basic principles of experimental/instrumental methods of analysis, and to execute them suitably for an in-depth analysis of chemical problems.

PSO 3: Skills to design and perform scientific experiments and to accurately record and analyze the experimental results.

PSO 4: Overall core competency in the subject and acquire skills for employment in academia and industry.

PSO 5: Knowledge relevant to the needs of present day society in regional, national and international development.

PSO 6: Professional skills to undertake chemical research in any societally relevant areas by inculcating the spirit of teamwork, innovation and entrepreneurship.

SEMESTER: 1

Semester Credit: 22(Core: 16; Elective: 6) Cumulative Credit:22

Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
24-341-0101	Inorganic Chemistry -I (Concepts and Developments)	Core	3	3-1-0	50	50	100
24-341-0102	Organic Chemistry-I (Reactivity and Mechanisms)	Core	4	4-1-0	50	50	100
24-341-0103	Theoretical Chemistry-I (Quantum Chemistry)	Core	3	3-1-0	50	50	100
24-341-0104	Theoretical Chemistry-II (Group Theory and Spectroscopy)	Core	4	4-1-0	50	50	100
24-341-0105	Advanced Chemical Synthesis and Separation Lab	Core	2	0-0-4	100	-	100
24-341-0106	Open Ended Lab-I	Core[a]	-	0-0-4	50	-	-
24-341-xxxx	Elective-1	Elective	3	3-1-0	50	50	100
24-341-xxxx	Elective-2	Elective	3	3-1-0	50	50	100
24-341-0111	Professional and Career Development in Chemistry	Audit [b]	-	2-0-0	-	-	-
List of Electives							
24-341-0107	Equilibrium Thermodynamics	Elective	3	3-1-0	50	50	100
24-341-0108	Environmental Chemistry	Elective	3	3-1-0	50	50	100
24-341-0109	Advanced Stereochemistry	Elective	3	3-1-0	50	50	100
24-341-0110	Polymer Chemistry	Elective	3	3-1-0	50	50	100

SEMESTER: 2

Semester Credit: 23 (Core: 20; Elective: 3) Cumulative Credit:45

Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
24-341-0201	Inorganic Chemistry-II (Chemistry of d- and f- Block Elements)	Core	3	3-1-0	50	50	100
24-341-0202	Organic Chemistry -II (Reactions, Reagents and Synthesis)	Core	4	4-1-0	50	50	100
24-341-0203	Organic Chemistry -III (Spectroscopy of Organic Compounds)	Core	3	2-1-0	50	50	100
24-341-0204	Physical Chemistry-I (Statistical and Nonequilibrium Thermodynamics)	Core	3	3-1-0	50	50	100
24-341-0205	Theoretical Chemistry-III (Chemical Bonding and Computational Chemistry)	Core	3	2-0-2	50	50	100
24-341-0206	Advanced Physical Chemistry Lab	Core	2	0-0-4	100	-	100
24-341-0207	Open Ended Lab-II	Core[a]	2	0-0-4	50	-	100[b]
24-341-xxxx	Elective -3	Elective	3	3-1-0	50	50	100
List of Electives							
24-341-0208	Bioanalytical Chemistry	Elective	3	3-1-0	50	50	100
24-341-0209	Advanced Photochemistry	Elective	3	3-1-0	50	50	100
24-341-0210	Theory of Orbital Interactions in Chemistry	Elective	3	3-1-0	50	50	100
24-341-0211	Transition Metals: Chemistry and Applications in Organic Synthesis	Elective	3	3-1-0	50	50	100
24-341-0212	New Methods and Strategies in Organic Synthesis and Dynamic Stereochemistry	Elective	3	3-1-0	50	50	100
24-341-0213	Materials Chemistry	Elective	3	3-1-0	50	50	100

SEMESTER: 3

Semester Credit: 19(Core: 16; Elective: 3) Cumulative Credit:64

Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
24-341-0301	Analytical Chemistry (Advanced Analytical Techniques and Instrumental Methods)	Core	4	4-1-0	50	50	100
24-341-0302	Inorganic Chemistry -III (Organometallic and Bioinorganic Chemistry)	Core	3	3-1-0	50	50	100
24-341-0303	Organic Chemistry-IV (Chemistry of Natural Products)	Core	3	3-1-0	50	50	100
24-341-0304	Physical Chemistry-II (Chemical Kinetics, Reaction Dynamics, Catalysis and Surface Chemistry)	Core	3	3-1-0	50	50	100
24-341-0305	Physical Chemistry-III (Advanced Electrochemistry)	Core	3	2-1-0	50	50	100
xx-xxx-xxxx	Interdepartmental Elective	Elective	3	3-1-0	50	50	100
24-341-xxxx		Interdepartmental Elective	3	3-1-0	50	50	100
List of Interdepartmental Electives							
24-341-0306	Spectroscopic Techniques	Interdepartmental Elective	3	3-1-0	50	50	100
24-341-0307	Introduction to Molecular Modeling in Chemistry	Interdepartmental Elective	3	3-1-0	50	50	100
24-341-0308	Advanced Techniques in Organic Synthesis: Theory and Practice	Interdepartmental Elective	3	3-1-0	50	50	100

SEMESTER: 4

Semester Credit: 16(Core: 12; Elective: 4) Cumulative Credit:80

Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
24-341-0401	Project Dissertation and Viva Voce	Core	12	-	-	300	300
24-341-0402	MOOC	Elective	4		0	100	100

Students are allowed to register for MOOC courses with ABC ID and complete credit requirements before the third semester and the credit will be added in the fourth semester. Students shall take one MOOC course of four credits or two courses of 2 credits approved by the Department Council for completing the credit requirements.

a- Sum of marks obtained in CE of Sem 1 and Sem 2

b- Value Added Course

L-T-P ≡ Lecture-Tutorial-Practical Hours

CE ≡ Continuous Evaluation; ESE ≡ End Semester Evaluation

CORE

24-341-0101

INORGANIC CHEMSISTRY-I

(CONCEPTS AND DEVELOPMENTS)

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O. 1: Identify the structure-activity relationship of simple molecules based on their qualitative molecular orbitals.	Analyse
C.O. 2: Predict the stability and topology of different polyhedral boranes and related compounds.	Analyse
C.O. 3: Assess the strength of various acids and bases and their reactivity.	Analyse
C.O. 4: Explain behavior of different non-aqueous solvent systems towards different reactions.	Apply
C.O. 5: Interpret the structure and properties of compounds of sulfur, nitrogen, phosphorous and group 14 elements.	Apply

	Programme Specific Outcomes					
Course Outcomes	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O.1	3	2	1	3	2	1
C.O.2	3	2	1	3	2	1
C.O.3	3	2	1	3	2	1
C.O.4	3	2	1	3	2	1
C.O. 5	3	2	1	3	2	1

UNIT – 1 **(10 hrs)**

Qualitative molecular orbital theory, symmetry of molecular orbitals, MOs for homo and heteronuclear diatomic molecules, H_2 to F_2, HF, CO, NO, BeH_2, CO_2,

H_2O, BH_3, NH_3, B_2H_6, $B_3N_3H_6$, S_3N_3, $N_3P_3Cl_6$, Si_2H_2. Importance of frontier molecular orbitals, Shape, energy and reactivity of molecules.

UNIT – 2 **(10 hrs)**

Electronic structure and allotropes of boron, boron halides, boron heterocycles, borazine Structure and bonding in polyhedral boranes and carboranes, styx notation; electron count in polyhedral boranes; Wade's rule; topological approach to boron hydride structure. Importance of icosahedral framework of boron atoms in boron chemistry. Closo, nido and arachno structures. Synthesis of polyhedral boranes; electron counting in polycondensed polyhedral boranes, mno rule. Carboranes, metallocarboranes; Boron halides, boron heterocycles, borazine.

UNIT – 3 **(10 hrs)**

Relative strength of acids, Pauling rules, Lux-Flood concept, Lewis concept, Generalized acid-base concept, Measurement of acid base strength, Lewis acid – base interactions, steric and solvation effects, acid–base anomalies, Pearson's HSAB concept, acid-base strength and hardness and softness, Symbiosis, theoretical basis of hardness and softness, electronegativity and hardness.

UNIT – 4 **(8 hrs)**

Chemistry in non-aqueous solvents reactions in NH_3, liquid SO_2, solvent character, reactions in SO_2, acetic acid, solvent character, reactions in H_2SO_4 and some other solvents. Molten salts, Green solvent: supercritical CO_2, Ionic liquids and deep eutectic solvents.

UNIT – 5 **(10 hrs)**

Sulphur-Nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl. SxNy compounds. S-N cations and anions. Sulphur-phosphorus compounds: Molecular sulphides such as P_4S_3, P_4S_7, P_4S_9 and P_4S_{10}. Phosphorus-nitrogen compounds: Phosphazenes and poly phosphazenes. Transition metal dichalcogenides, MoS_2. Structure, bonding and reactivity of 2D and 3D Carbon, Silicon and Germanium materials. Carbon nitrides, fullerenes, carbon nanotubes

(CNT's) and graphenes.

Recommended Text Books:

1. G.L. Miessler, P.J. Fischer, D.A. Tarr, Inorganic Chemistry, 5th ed., Pearson, 2014.
2. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.
3. F. A. Cotton, G. Wilkinson, C. A, Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th ed., Wiley-Interscience: New York, 1999.
4. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd ed., ELBS, 1999.
5. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd ed., Wiley, 1994.
6. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd ed., Butterworth-Heinemann, 1997.
7. C.E. Housecroft, A.G. Sharpe, Inorganic Chemistry, 5th ed., Pearson, 2018.
8. E. Wiberg, A.F. Holleman, N. Wiberg, Inorganic Chemistry, Academic Press,2001.
9. A. V. Kolobov, J. Tominaga, Two-Dimensional Transition Metal Dichalcogenides, Springer, 2016.
10. Yu-Chuan Lin, Properties of Synthetic Two-dimensional Materials and Heterostructures, Springer, 2018.
11. Changzheng Wu, Xiaojun Wu, et al, Inorganic Two-dimensional Nanomaterials: Fundamental Understanding, Characterization and Energy Applications, RSC, 2017
12. D.R. MacFarlane, Mega Kar, J.M. Pringle, Fundamentals of ionic liquids, Wiley-VCH, 2017.
13. Yizhak Marcus, Deep Eutectic Solvents, Springer, 2019.
14. J.M. DeSimone and W. Tumas, Green Chemistry Using Liquid and Supercritical Carbon dioxide, D.U.P, 2003.
15. F. M. Kerton , R. Marriott , et al., Alternative Solvents For Green Chemistry, 2nd ed., RSC, 2013.

CORE

24-341-0102

ORGANIC CHEMISTRY -I

(REACTIVITY AND MECHANISMS)

Credit 4 **64 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Apply methods and techniques to study mechanisms of organic reactions.	Apply
C.O.2: Propose a reasonable mechanism for a given organic reaction.	Evaluate
C.O.3: Predict the products in a particular reaction considering the stereochemical aspect.	Evaluate
C.O.4: Illustrate the mechanistic pathway of different rearrangement and pericyclic reactions.	Analyse
C.O.5: Identify the mechanism and the product in a given reaction under photochemical condition.	Analyse

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	1	0	3	3	1
C.O.2	3	1	0	3	3	1
C.O.3	3	1	0	3	3	1
C.O.4	3	1	0	3	3	1
C.O.5	3	1	0	3	3	1

UNIT – 1 **(10 hrs)**

The study of reactions and the methods of studying reaction mechanisms. Classification of reactions according to IUPAC conventions. Reaction mechanism: guidelines on Pushing of electrons. Reactive intermediates:

Formation, stability and general reactivity. Methods of determining reaction mechanisms (kinetic and non- kinetic methods): The Hammond postulate, reactivity vs selectivity principle, the Curtin-Hammett principle, microscopic reversibility, kinetic vs thermodynamic control. Isotope effects: Primary, secondary and Equilibrium isotope effects, Tunneling effects, solvent isotope effects and heavy atom Isotope effects.

Linear free energy relationships: Hammett and Taft parameters, Solvent effects (Grunwald-Winstein plots and Schleyer adaptation), nucleophilicity and nucleofugality. Isokinetic and Isoequilibrium temperature, Enthalpy – entropy compensation. Experimental techniques to determine reaction mechanisms: identification of intermediates by trapping and competition experiments, cross - over experiments, isotope scrambling, radical clocks and traps, matrix isolation

UNIT – 2 **(14 hrs)**

Substitutions on Aliphatic carbon – saturated and unsaturated systems – Mechanism of nucleophilic substitution – SN2, SN1 – ion pairs, SET, Neighbouring group participation – non classical carbocations, SNi, Tetrahedral mechanism. Electrophilic substitution – SE2, SEi, SE1. Free radical substitution. Reactivity – Effect of substrate structure, nature of reagents, solvents and stereochemistry on the outcome of these reactions. Ambident nucleophiles and substrates. Typical reactions involving substitution.

Substitutions on aromatic carbon: Mechanism of electrophilic, nucleophilic and free radical substitutions – orientation and reactivity. Typical reactions involving aromatic substitution.

UNIT – 3 **(16 hrs)**

Mechanisms of polar addition – electrophilic, nucleophilic and free radical addition. Nonpolar additions (excluding pericyclic reactions) - Reactivity and orientation. Eliminations - E2, E1 and E1CB mechanisms, reactivity and orientation. Pyrolytic syn eliminations, α - eliminations, elimination vs. substitution. Typical reactions involving addition and elimination.

Rearrangements involving electron deficient carbon and nitrogen. Mechanism of the following rearrangements: Wagner-Meerwein, Pinacol, Demyanov, dienone-phenol, Favorskii, Wolff, Hofmann, Curtius, Lossen, Schmidt, Beckmann, benzidine, and Hofmann-Loffler, Fries, Baeyer-Villiger rearrangements. Fritsch-Buttenberg-Wiechell rearrangement,Corey-Fuchs reaction, Seyferth-Gilbert homologation, Grubbs catalysts and olefin metathesis.

UNIT – 4 (14 hrs)

Pericyclic reactions: study of the principle of conservation of orbital symmetry: Orbital symmetry diagrams for cycloaddition and electrocyclic reactions. Aromatic Transition State Theory and The Generalized Woodward – Hoffmann rule applied to cycloadditions, Electrocyclic reactions, Sigmatropic rearrangements and Chelotropic reactions.

Pericyclic Reactions in Organic Synthesis: Stereochemistry and Regiochemistry of Cycloadditions. Substituent and medium effects, Secondary Orbital Interactions in [4+2] cycloadditions, Intramolecular Diels–Alder reactions. Stereochemistry of Electrocyclic Reactions and Sigmatropic rearrangements. Cope rearrangement, Claisen rearrangement and ene-reaction.

1,3-dipolar cycloaddition reactions, Photochromism and thermochromism, Pericyclic reactions in Organic synthesis – case studies.

UNIT – 5 (10 hrs)

Photochemistry: Unimolecular and bimolecular processes in the excited states, mechanism of important photochemical reactions, Paterno-Buchi reaction, Norrish Type I and Type II fragmentation, di-pimethane rearrangement, Barton reaction, photochemistry of olefins, arenes, cyclohexadienones; photoreduction and photo-oxygenation.

Recommended Text Books:

1. J. March, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed., Wiley, 2013.
2. T. H. Lowry, K. S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd ed., Benjamin-Cummings Publishing Company, 1997.

3. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.

4. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry. University Science Books, 2006.

5. F. A. Carroll, Perspectives on structure and mechanism in Organic Chemistry,Wiley, 2011.

6. N. S. Issacs, Physical Organic Chemistry, 2nd Edition, Prentice Hall, 1995.

7. A. Pross, Theoretical and Physical Principles of Organic Chemistry, 1st ed., Wiley, 1995.

8. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.

9. J. McMurry, Organic Chemistry, 5th ed., Brooks/Cole, 2000.

10. R. Bruckner, Advanced organic chemistry: Reaction Mechanisms. Academic Press, 2001.

11. P. Sykes, Guidebook to Mechanism in Organic Chemistry, 6th ed., Prentice Hall, 1986.

12. N. J. Turro, Modern Molecular Photochemistry, University Science Books, 1996.

13. N. J. Turro, J. C. Scaiano, V. Ramamurthy, Modern Molecular Photochemistry of Organic Molecules, 1st ed., University Science Books, 2010.

CORE

24-341-0103

THEORETICAL CHEMISTRY-I
(QUANTUM CHEMISTRY)

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Describe and justify the importance of Quantum Mechanics by applying various postulates in deriving property operators and Schrodinger equation	Analyse
C.O.2: Apply the postulates of quantum mechanics to systems of chemical interest, such as the particle-in-a-box, harmonic oscillator, rigid rotor, hydrogen atom and multielectronic atoms and interpret the results.	Apply
C.O.3: Derive the variational principle and perturbation theory, use them to calculate properties for simple systems of chemical interest	Analyse
C.O.4: Define and explain the Hartree-Fock self-consistent field method.	Apply

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	1	0	2	1	0
C.O.2	3	1	0	3	1	0
C.O.3	2	1	0	2	1	0
C.O.4	3	1	1	3	1	1

UNIT – 1 **(10 hrs)**

Wave-particle duality, uncertainty principle, postulates of quantum mechanics, Schrödinger equation, Time dependent and time independent Schrodinger wave equation. Its application on some model systems viz., free particle, particle in one, two and three-dimensional box (rectangular and cubical), separation of variables, concept of degeneracy, introduction to quantum mechanical tunneling.

UNIT – 2 **(10 hrs)**

Vibrational motion, Harmonic oscillator, Method of power series, Hermite equation and Hermite Polynomials, Recursion formula, wave function and energy. Rigid rotator, Wave function in spherical polar coordinates, Planar rotator, phi equation, theta equation and solutions Lagendre equation and Lagendre polynomials, Spherical harmonics, Angular momentum operator L^2 and L_z, Space quantization.

UNIT – 3 **(10 hrs)**

H atom, separation into three equations and solutions, Laguerre equation and Laguerre polynomials wave equation and energy of H like systems, quantum numbers and their importance, Radial wave function and radial distribution functions, angular wave function, Shapes of s, p, d and f atomic orbitals.

Postulate of electron spin-orbital and spin functions. Zeeman effect.

UNIT – 4 **(12 hrs)**

Many electron atoms. Approximate methods in quantum mechanics: The variation theorem, linear variation principle and perturbation theory (first order and non- degenerate), application of variation method and perturbation theory to the Helium atom, antisymmetry, Pauli exclusion principle, Slater determinantal wave functions. Electron spin.

UNIT – 5 **(6 hrs)**

Hartree-Fock Self Consistent Field method, The Coulomb and Exchange Operators, The Fock Operator, Koopmans' theorem, Brillouin's theorem, The Roothaan Equations, Slater's treatment of complex atoms, Slater orbitals. Pauli principle, Slater determinant and wave function.

Recommended Text Books:

1. D. A. McQuarrie, Quantum Chemistry, 3rd ed., Univ. Sci. Books, Mill Valley, California, 1983.
2. I. N. Levine, Quantum Chemistry, 6th ed., Pearson Education, London, 2008.
3. P. W. Atkins, R.S Friedman, Molecular Quantum Mechanics, 5th ed., OUP, Oxford, 2012.
4. J. P. Lowe, Quantum Chemistry 3rd ed., Academic Press, New York, 2008.
5. A. Szabo, N. S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Book ed., Mc.Graw-Hill, New York, 1982.
6. P.W. Atkins, Physical Chemistry, 8th ed., Wiley, New York, 2006.
7. R. K. Prasad, Quantum Chemistry, 3rd ed., New Age International, 2006.
8. D. J. Griffiths, Introduction to Quantum Mechanics, 2nd ed., 2004.
9. J. J. Sakurai, Modern Quantum Mechanics, 2nd ed., 2010.

CORE

24-341-0104

THEORETICAL CHEMISTRY-II

(GROUP THEORY AND SPECTROSCOPY)

Credit 4 **64 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O. 1: Analyze the symmetry of any given molecule and assign the point group	Analyze
C.O.2: Apply the principles of symmetry and group theory in structure, bonding and spectral characteristics of molecules	Apply
C.O.3: Explain the factors affecting the intensity and broadening of lines in spectra and methods to enhance the sensitivity	Understand
C.O.4: Explain the principles of rotational, vibrational, Raman, electronic, fluorescence and NMR spectroscopy	Understand
C.O.5: Solve problems based on rotational, vibrational, Raman electronic, fluorescence and NMR spectroscopy	Apply
C.O.6: Apply various theoretical aspects to various spectroscopic techniques for prediction of different spectroscopic observations	Analyze

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	3	1	3	2	1
C.O.2	3	3	1	3	2	1
C.O.3	3	3	1	3	3	2
C.O.4	3	3	1	3	3	2
C.O. 5	3	3	1	3	3	2
C.O. 6	3	3	1	3	3	2

UNIT – 1 **(16 hrs)**

Matrix representation of symmetry operations, similarity transformation and classes, Symmetry classification of molecules into point groups (Schoenflies symbol)- Application of symmetry topredict polar and chiral compounds. Reducible and Irreducible representations - Great Orthogonality theorem and its consequences (statement only, proof not needed), Character tables, Reduction formula, construction of character tables for point groups with order ≤6, Interpretation of character tables. Wave functions as bases for irreducible representations, Direct product.

UNIT – 2 **(10 hrs)**

Application of symmetry to predict polar and chiral compounds. Application of Group theory to Hybridization of atomic orbitals: Construction of hybrid orbitals for AB_3(planar), AB_4(T_d), AB_5(D_{3h}) and AB_6(O_h) type of molecules.

Application of group theory to Molecular Orbital Theory: LCAO and Huckel approximations. Symmetry adapted linear combinations, Projection operators, Application of projection operators to pi-bonding in ethylene, cyclopropenyl systems, benzene and naphthalene. Application of projection operators to sigma bonding in ethylene and $PtCl_4^{2-}$. Molecular orbitals for tetrahedral and octahedral molecules.

UNIT – 3 **(10 hrs)**

Spectroscopy and its importance in chemistry. Link between spectroscopy and quantum chemistry, Energy levels in molecules, Born-Oppenheimer approximation, Absorption and emission of radiation, Intensity and width of spectral lines, Beer lambert's law, Integrated absorption coefficient, Line width – natural line broadening, Doppler broadening, minimisation of line broadening, Induced and spontaneous transitions, correlation to the Einstein coefficients of absorption and emission, Basis of selection rules Fermi golden rule, lasers.

UNIT – 4 **(14 hrs)**

Rotational spectroscopy: Rotation of rigid bodies, moment of inertia, linear molecules, spherical, symmetric and asymmetric tops, Schrödinger equation of a rigid rotator and brief discussion of its results, Quantization of rotational energy levels, selection rules, rotational spectra and line intensities, structure determination from rotational constants, isotopic effects.

Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results, concept of zero-point energy. Quantization of vibrational energy levels. Selection rules, IR spectra of diatomic molecules. Structural information derived from vibrational spectra, dissociation energies, vibration-rotation transitions in diatomics, harmonic oscillator, anharmonicity, centrifugal distortion, Vibration of polyatomic molecules, normal modes, combination, difference and hot bands, Fermi Resonance, Group frequencies. Effect of hydrogen bonding (inter- and intramolecular) on vibrational frequencies.

Raman spectroscopy: Light scattering and Raman effect, classical and quantum models for scattering, Stokes and anti-Stokes lines; their intensity difference, polarizability, selection rules, group theoretical treatment of vibrations, Effect of nuclear spin, Vibrational Raman spectra, rule of mutual exclusion for centrosymmetric molecules, polarized and depolarized Raman lines, resonance Raman scattering.

Applications of Group theory for molecular vibration, symmetry of group vibrations. Selection rules and applications to IR and Raman spectra.

UNIT – 5 **(14 hrs)**

Electronic Spectroscopy of molecules: Molecular orbitals and states, term symbols, selection rules, vibrational and rotational structures, Free Electron model, its application to electronic spectra of polyenes. Frank-Condon principle, electronic transitions, Beer Lambert's Law, dissociation and predissociation, photoelectron spectroscopy, dissociation and predissociation, calculation of heat of dissociation, Birge Sponer method, electronic spectroscopy of polyatomic molecules

Singlet and triplet states, Jablonski diagram, fluorescence and phosphorescence, Solvent and environmental effects, Fluorescence quenching, energy transfer and electron transfer, time domain lifetime measurements.

NMR: Expression for Hamiltonian/Energy - Zeeman interaction, torque exerted by a magnetic field on spins, equation, its solution and the physical picture of precession. Thermal equilibrium, Relaxation, chemical shift, shielding and deshielding, Karplus relationships, Bloch equations, the rotating frame, pulsed experiments, NOE, double irradiation, selective decoupling, double resonance, Polarisation transfer, Two-dimensional NMR, Solid state NMR, NQR, MRI.

Recommended Text Books:

1. F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern, Singapore, 2nd ed., 1992.

2. V. Ramakrishnan, M. S. Gopinathan, Group theory in Chemistry, Vishal Pub. New Delhi, 1996.

3. Alan Vincent, Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd ed., Wiley, 2013.

4. Robert L. Carter, Molecular Symmetry and Group Theory, Wiley, 2009.

5. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1962.

6. C. N. Banwell, Fundamentals of Molecular Spectroscopy, 4th ed., Tata McGraw Hill, 1996.

7. A. E. Derome, Modern NMR Techniques for Chemical Research, Pergamon Press, 1987.

8. D. H. Williams, I. Flemming, Spectroscopic Methods in Organic Chemistry, 4th ed., McGraw-Hill, 1985.

9. H. Gunther, NMR Spectroscopy, 2nd ed., John Wiley, 2005.

10. N. B. Colthup, L. H. Daly, S. E. Wiberley, Introduction to Infrared and Raman Spectroscopy, 3rd ed., 1982.

11. R. A. Alberty, Physical Chemistry 8th ed., Wiley, New York, 1994.

12. P. W. Atkins, Physical Chemistry 8th ed., W. H. Freeman, New York, 2006.

13. I. N. Levine, Molecular Spectroscopy, John Wiley & Sons.

14. J. M. Hollas, Modern Spectroscopy, John Wiley & Sons.

15. P. F. Bernath, Spectra of Atoms and Molecules, III Edn, Oxford University Press.

16. J. L. McHale Molecular Spectroscopy, Pearson Education.

17. W. W. Parson, Modern Optical Spectroscopy, Springer-Verlag.

18. Jack D. Graybeal, Molecular Spectroscopy, Mc Graw Hill International Editions

19. M.H. Levitt, Spin Dynamics, II edn.Wiley

20. James Keeler, Understanding NMR spectroscopy, II edn. Wiley

21. Joseph R. Lakowicz, Principles of Fluorescene Spectroscopy, 3rd Ed., Plenum Press, 2010.

CORE

24-341-0105

ADVANCED CHEMICAL SYNTHESIS AND SEPARATION LAB

Credit 2 **64 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Acquire knowledge on safe laboratory practices of handling laboratory glassware, equipment and chemical reagents.	Knowledge
C.O.2: Plan and perform synthetic procedures, chromatographic separation and purification of organic compounds.	Understand
C.O.3: Separate organic compounds from the organic binary mixture and identify the functional group(s) present.	Analysis
C.O.4: Use software to Draw the structures and schemes of organic molecules and reactions.	Apply
C.O.5: Use Chemical Abstracts, Scopus, Organic Synthesis collective volumes on web etc. to search, analyse and collect chemical information.	Apply
C.O.6: Identify the cations in a mixture of unknown salts.	Analyse
C.O.7: Estimate the amount of a given metal ion by complexometric and cerimetric reactions.	Analyse
C.O.8: Synthesise metal complexes and characterize them by various physicochemical methods.	Apply
C.O.9: Record and interpret electronic spectrum of different metal complexes.	Apply

	Programme Specific Outcomes					
Course Outcomes	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O.1	3	3	3	3	3	3
C.O.2	3	3	3	3	3	3
C.O.3	3	3	3	3	3	3
C.O.4	3	3	3	3	3	3
C.O.5	2	3	3	3	2	3
C.O.6	2	3	3	2	3	3
C.O.7	3	3	3	3	3	3
C.O.8	3	3	3	3	2	3
C.O.9	3	3	3	2	3	3

UNIT – 1 **(34 hrs)**

Part I: General methods of separation and purification of Organic compounds such as 1) Solvent extraction 2) Thin layer chromatography and paper chromatography

3) column chromatography

Part II: Separation and identification of the components of organic binary mixtures.

Part III: Preparation of Organic compounds by multistep reactions, purification of products and characterisation using UV-Vis, FTIR and NMR.*

Part IV: Drawing the structures of organic molecules and reaction schemes by Proprietary and open source computer software. Use Chemical Abstracts, Scopus, Organic Synthesis collective volumes on web etc., to search, analyse and collect chemical information.

*Progress of the reactions should be followed by spectroscopic and chromatographic methods (UV-Vis, TLC, GC, HPLC, etc)

UNIT – 2 **(30 hrs)**

Reactions of titanium, vanadium, chromium, manganese, iron, cobalt, nickel and copper ions. Reactions of some less common metal ions (Tl, W, Mo, V, Zr, Th, U). The spot test technique for metal ions. Semimicro qualitative analysis of common and rare cations in a mixture.

Estimation of metal ions by complexometric and cerimetric titrations. Estimation of Mg, Ca, Mn, hardness of water.

Synthesis of inorganic complexes and their characterization by various physicochemical methods, such as IR, UV, Visible, NMR, magnetic susceptibility etc. Selection can be made from the following or any other complexes for which references are available in the literature.

Tris(oxalato)manganese(III)

Tetrapyridinesilver(II)peroxidisulphate

Tris(acetylacetonato) iron(III)

Bis(N,N-diethyldithiocarbamato)nitrosyliron(I)

Optical isomers of tris(ethylenediamine)cobalt(III)chloride

Nitropentamminecobalt(III) chloride

Tri(acetylacetonato)manganese(III)

Tris(thiourea) copper(I) sulphate

Phenyl lithium

Tetraphenyl lead

Ferrocene

Phosphonitrilic chloride

Anhydrous copper(II) nitrate

Interpretation of its electronic spectrum and calculation of Dq values.

Determination of crystal field splitting energy for certain ligands and construction of a part of the spectrochemical series.

Recommended Text Books:

1. A. I. Vogel, A. R. Tatchell, B. S. Furnis, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, 5th ed., John Wiley, 1989.
2. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Organic laboratory Techniques, 3rd ed., Saunders Golden Sunburst Series.
3. L. W. Harwood, C. J. Moody, Experimental Organic Chemistry-Principles and Practice, Blackwell Science Publications.
4. G. Pass, H. Sutcliffe. Practical Inorganic Chemistry 2nd ed., Chapman & Hill. 1974.
5. G. Marr, B. W. Rockett, Practical Inorganic Chemistry, Van Nostrand, 1972.

CORE/LAB

24-341-0106

OPEN ENDED LAB-I

Credit 0 **32 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Design experiments and validate the hypothesis of an independent research problem.	Evaluate

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	2	2	3	3	2	3

UNIT – 1

The students shall perform literature review/ experiments/analysis for validating the hypothesis and Submit Research Proposal

ELECTIVE

24-341-0107

EQUILIBRIUM THERMODYNAMICS

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O. 1: To predict changes in thermodynamic parameters during a process and predict the spontaneity.	Apply
C.O. 2: Describe the significance of chemical potential in physical and chemical processes	Apply
C.O. 3: Understand thermodynamics of phase transitions and interpret phase diagram of a given system.	Analyse
C.O. 4: Interpret dependence of chemical equilibrium on pressure, temperature and concentration.	Analyse

	Programme Specific Outcomes					
Course Outcomes	**P.S.O 1**	**P.S.O 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O 5**	**P.S.O. 6**
C.O.1	3	3	2	3	3	3
C.O.2	3	3	2	3	3	3
C.O.3	3	3	2	3	3	3
C.O.4	3	3	2	3	3	3

UNIT – 1 **(8 hrs)**

Language and Mathematics of Thermodynamics.

Recap of first and second law. The Clausius inequality, Free energy functions - Variation with temperature and pressure. Gibbs Helmholtz equation. Relation between thermodynamic functions. Maxwell relations-significance.

Third law of thermodynamics: Nernst Heat Theorem, Calculation of absolute entropy, Unattainability of absolute zero.

UNIT-2 **(10 hrs)**

Thermodynamic systems of variable composition – Partial molar properties. Chemical Potential, Significance of Chemical potential, Gibbs Duhem Equation and Duhem Margules Equation. Thermodynamics of mixing. Excess functions, Concepts of activity and fugacity, Standard states.

UNIT – 3 **(10 hrs)**

Physical transformation of Pure substances- Stability of a phase, Phase transitions and phase boundaries- Thermodynamic aspects, Ehrenfest Classification of Phase transitions. Phase rule – Application to one component systems- Water, S, CO_2 and He.

UNIT – 4 **(10 hrs)**

Thermodynamics of Binary systems: Binary liquids- Ideal solutions, Raoults law, Henry's Law, Deviations from ideality, Real and Regular solutions, Excess functions, Ideal Dilute Solutions- Colligative Properties- van't Hoff factor.

Liquid-vapour equilibria of binary systems – Vapour pressure-composition diagrams and Temperature composition diagrams. Distillation of binary mixtures –Azeotrope formation.

Liquid-liquid equilibria- Partially miscible and immiscible liquids- CST, Nernst Distribution Law, Partition co-efficient, Principle of Steam distillation.

Solid-liquid Equilibria-Cooling curve, Eutectic system, Deep Eutectic solvents, Application, Compound formation with Congruent and Incongruent melting points. Salt hydrate water systems,

Solid-Vapour Equilibria- CuSO4-water system. Three component systems.

UNIT – 5 **(10 hrs)**

Chemical Equilibria and free energy, Equilibrium Constants, Applications of free energy function to physical and chemical changes- Le Chateliers Principle. Effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isotherm and isochore.

Recommended Text Books:

1. Peter Atkins and Julio de Paula, Physical Chemistry, Oxford University Press, 8^{th} and10^{th} Edn, 2017.

2. D.A.McQuarrie, J.D Simon, Molecular Thermodynamics, Viva Student Edn. 2010.
3. I.N Levine, Physical Chemistry, McGraw Hill Indian Edn, 2011.
4. I.M.Klotz & R. M. Rosenberg, Chemical Thermodynamics, Wiley, 7th Edn, 2008.
5. L.K.Nash, Elements of Chemical Thermodynamics, Addison Wesley, 2nd Edn, 2013.
6. F.Daniels and R. A. Alberty, Physical Chemistry, Wiley Publishers, 4th Edn 2004

ELECTIVE

24-341-0108

ENVIRONMENTAL CHEMISTRY

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O. 1: Explain various cycles in environment	Understand
C.O. 2: Identify various air, soil and water pollutants andsuggest methods to control air, water and soil pollutions	Apply
C.O. 3: Discuss the various techniques in environmentalanalysis	Apply

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	1	0	2	1	0
C.O.2	3	1	1	2	1	1
C.O.3	3	1	1	2	1	1

UNIT – 1 **(8 hrs)**

Global warming – Ozone hole. Environmental segments – The hydrological cycle – The oxygen cycle – The nitrogen cycle – The sulphur cycle – Composition of atmosphere – Earth's radiation balance – Green house effect.

UNIT – 2 **(10 hrs)**

Air pollution – Primary pollutants, Acid rain – Air quality standards – Sampling – Monitoring – Analysis of CO, nitrogen oxides, sulphur oxides, hydrocarbons and particulate matter – Control of airpollution.

UNIT – 3 **(10 hrs)**

Soil pollution – Inorganic and organic components in soil – Acid – Base and ion exchange reactions in soils – Micro and macro nutrients – Wastes and pollutants in soil.

UNIT – 4 **(10 hrs)**

Water pollution – Water pollutants – Eutrophication – Water quality criteria for domestic and industrial uses – Trace elements in water – Determination of quality parameters – Total hardness, TDS, pH, chloride, heavy metals, etc.

Principles of water and waste water treatment – Aerobic and anaerobic treatment – Industrial waste water treatment – Removal of organic and inorganic materials from water and waste water.

UNIT – 5 **(10 hrs)**

Instrumental techniques in environmental analysis – Use of neutron activation analysis – ASV, AAS, GC, HPLC, ion selective electrodes and ion chromatography in environmental chemical analysis.

Recommended Text Books:

1. Environmental Chemistry, Gary W. VanLoon, Stephen J. Duffy, Oxford University Press,2005
2. Principles of Environmental Chemistry, James Girard, Jones & Bartlett Learning,2005
3. Environmental Chemistry, Seventh Edition, Stanley E. Manahan, CRC Press,2010
4. Applications of Environmental Chemistry, Eugene R. Weiner, CRCPress,2010
5. Environmental chemistry, Ian Williams, J. Wiley, 2001
6. The essential guide to environmental chemistry, Georg Schwedt, John Wiley,2010

ELECTIVE

24-341-0109

ADVANCED STEREOCHEMISTRY

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Understand the concept of Configuration and conformation of organic compounds	Understand
C.O.2: Apply the concepts of conformation and configuration in organic chemistry.	Apply
C.O.3: Apply the concepts of stereochemistry and conformation chemistry of carbohydrates	Apply
C.O.4: Analyze the effect of molecular conformation in the outcome of a reaction.	Analyze

	Programme Specific Outcomes					
Course Outcomes	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O.1	3	3	1	3	2	1
C.O.2	3	2	1	2	2	1
C.O.3	3	2	1	2	2	2
C.O.4	3	3	1	3	2	1

UNIT – 1 **(8 hrs)**

Geometrical isomerism, origin – structural features including C-C and C-hetero atom double bonds, cyclic systems and other systems exhibiting restricted rotation, different nomenclature including, *cis-tarns*, *E-Z, syn-anti*, *endo-exo, in-out*, relative acidity of maleic and fumaric acids.

UNIT – 2 **(10 hrs)**

Optical isomerism, origin of chirality, chiral centres, axes and planes, helicity, enantiotopic and diastereotopic atoms, groups and faces, prochiral centres and faces, allenes, cumulenes, biphenyls, and spirans. Compounds containing chiral atoms other than carbon.

Brief introduction to CD and ORD techniques, octant rule, axial haloketone rule, and sign of Cotton effect

UNIT – 3 **(10 hrs)**

Conformational analysis, Acyclic sp^3–sp^3, sp^3-sp^2 systems, structure and stability of small, medium, and large rings, cyclohexane, substituted cyclohexanes, *A*values, cyclohexenes, decalins, bicyclic systems. Strain, types of strain including *B*, *F*, *I*, Pitzer strain, Beyer strain.

UNIT – 4 **(10 hrs)**

Conformation and Stereo-electronic Effects of carbohydrates: *D* and *L* sugars, Chair conformation, Endo/Exo-anomeric effect, Reverse anomeric effect, Glycosidic torsion angles, Hydroxymethyl group conformation. Conformationand stability of aldohexoes, structure and conformation of ribose and deoxyribose.

UNIT – 5 **(10 hrs)**

Reaction Mechanisms and Conformational Effects on Reactivity - EsterHydrolysis, Alcohol Oxidations, S_N2 Reactions, Elimination Reactions, Epoxidation by Intramolecular Closure of Halohydrins, Epoxide Openings (S_N2), Electrophilic Additions to Olefins, Rearrangement Reactions, Conformationaland Stereoelectronic Effects on Reactivity.

Stereoselective Reactions of cyclic compounds. Reactions on Small Rings. Stereochemical Control in Six Membered Rings. Stereochemistry of Bicyclic Compounds. Reactions with Cyclic Intermediates/Transition states.

Recommended Text Books:

1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 8th Ed., Wiley, 2020.
2. T H. Lowry and K.S. Richardson: Mechanism and Theory in Organic Chemistry, 3rd Ed., Benjamin-Cummings Publishing Company, 1997.
3. F. A. Carey and R. J. Sundberg: Advanced Organic Chemistry (parts A and B), 5th Ed., Springer, 2010.
4. E. V. Anslyn and D. A. Dougherty: Modern Physical Organic Chemistry. Ist Ed., University Science Books, 2011.
5. F. A. Carroll: Perspectives on structure and mechanism in organic chemistry, 2nd Ed., Wiley, 2011.
6. N. S. Issacs: Physical Organic Chemistry, 2nd Ed., Prentice Hall, 1995.
7. A. Pross: Theoretical and Physical Principles of Organic Chemistry, Ist Ed., Wiley, 1995.
8. J. Clayden, N. Green, S. Warren and P. Wothers: Organic Chemistry, 2nd Ed., Oxford University Press, 2012.
9. P.S.Kalsi: Stereochemistry, Conformation and Mechanism, 9th Ed., New Age Publications, 2017.
10. E. L. Eliel and S. H. Wilen: Stereochemistry in Organic Compounds, 2008, John Wiley.
11. S. H. Pine: Organic Chemistry, 5th Ed., McGraw Hill, 2008.
12. I. Flemming: Molecular orbitals and organic chemical reactions, student edition, 2009, Wiley.
13. J. McMurry, Organic Chemistry, 9th Ed., 2015, Brooks/Cole .
14. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 4th Ed., Wiley Eastern Limited, New Delhi, 2012.
15. Eliel, E. L. and Wilen, S. H. Stereochemistry in Organic Compounds, Student Ed., John Wiley, 2008.

ELECTIVE

24-341-0110

POLYMER CHEMISTRY

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
CO 1: To gain basic knowledge about various Polymerization mechanism	Understand
CO 2: To understand various types of polymerisation techniques and processing.	Analyse
CO 3: To get knowledge on polymer characterization	Analyse
CO 4: To get an idea about the functional polymers and the applications for advanced technologies	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	0	0	3	2	2
CO2	3	0	0	3	2	2
CO3	3	0	0	3	3	2
CO4	3	0	0	3	3	2

Unit I **(8 hrs)**

Introduction. Nomenclature. Classification. Molecular weight. Physical states. Crystalline and amorphous behaviour. Thermal transition. Mechanical properties. Chemical Bonding and Polymer Structure.

Unit II **(12 hrs)**

Polymerization Mechanism. Free radical addition polymerization. Kinetics and mechanism.

Chain transfer. Molecular weight distribution and molecular weight control. Cationic and anionic polymerization. Polymerization without termination. Living polymers. Step Growth polymerization. Kinetics and mechanism. Linear Vs cyclic polymerization, Group Transfer, metathesis and ring opening polymerization. Copolymerization. Copolymerization equation, Q-e scheme, Gelation and Crosslinking.

Unit III (8 hrs)

Polymerization techniques and Processing. Bulk Solution, melt, suspension, emulsion and dispersion techniques. Elastomers. Fibers. Plastics.

Unit IV (10 hrs)

Polymer Characterization. Molecular weights. Concept of average molecular weights, Determination of molecular weights. Gel Permeation Chromatography and Light scattering techniques. Molecular weight distribution. Crystalline and amorphous states. Glassy and Rubbery States. Glass transition and crystalline melting. Degree of Crystallinity, X-Ray diffraction analysis. Thermal analysis of polymers. TG/DTG, DTA/DSC, Spectroscopy of polymers. Microstructure determination by IR, Raman, UV, NMR and MS techniques. Solid State NMR.

Unit V (10 hrs)

Functional Polymers. Porous Organic Polymers, Covalent organic framework, Dendritic polymers, Conducting polymers, Redox polymers, Luminescent polymers. Liquid Crystalline polymers.Industrial polymers. Polyethylene, polystyrene. PVC, PAN, Poly(vinyl carbazole). Silicone polymers. Polymers for Advanced Technologies. Sensor Applications. Applications in Electronics and Energy – Electrically Conductive Polymers, Polymeric Batteries, Organic Photovoltaic Polymers. Photonic Polymers – Nonlinear Optical polymers, Light Emitting Diodes.

Recommended Books :

1. F. W. Billmeyer Jr., Textbook of Polymer Science, John Wiley and Sons, N.Y. 1991.

2. V. R. Gowarikar, Polymer Chemistry, New Age International Pvt. Ltd., New Delhi, 2010

3. George Odian, Principles of Polymerization, 4th Edn., Wiley, 2004

2. J.M.G Cowie. Polymers, Physics and Chemistry of Modern Materials. Blackie. London, 1992.

3. R.J.Young, Principles of Polymer Science, 3rd ed., Chapman and Hall. N.Y. 1991.

4. R. O. Ebewele, Polymer Science and Technology, CRC Press. N.Y., 1996

5. P.J. Flory, A Text Book of Polymer Science, Cornell University Press, Ithacka, 1953.

6. F. Ullrich, Industrial Polymers, Kluwer, N.Y, 1993.

7. H.G.Elias, Macromolecules, Vol. I & II, Academic, N.Y. 1991.

8. J.A.Brydson, Polymer Chemistry of Plastics and Rubbers, ILIFFE Books Ltd., London, 1966

9. J.R.Fried, Polymer Science and Technology, Pearson Education Inc., New Jersey, 2014.

AUDIT

24-341-0111

PROFESSIONAL AND CAREER DEVELOPMENT IN CHEMISTRY

Credit 0 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O. 1: Skills on subject specific pedagogy, soft skills, ICT tools, research proposal writing, finding scholarships and software for chemistry	Create

	Programme Specific Outcomes					
Course Outcomes	P.S.O.1.	P.S.O.2	P.S.O.3	P.S.O.4	P.S.O.5	P.S.O.6
C.O.1	1	2	3	3	3	1

UNIT – 1 **(48 hrs)**

Soft Skills – Powerpoint, Word, Exel, Reference management software- Mendeley, Origin, Veusz, Research Proposal Writing – Literature review, Components of proposals, ICT – Google Classroom, Moodle, Class Recording, Teach Infinity, OBS, edmondo, QUIZZ Quiz, Document scanner., Subject specificpedagogy – Molecular model kit, ChemDraw, ChemSketch, Finding International Scholarships- MEXT, DAAD, EURAXESS, J-Rec, Funding through embassy, Research ethics , research methodology, lab safety.

Recommended Text Books:

1. John M. Swales & Christine B. Feak, Academic Writing for Graduate Students 3rd Edition, Michigan Publishing, 2012

2. Stephen Bailey, Academic Writing, A Handbook for International Student,5th Edition, Routledge, Taylor & Francis,2018

CORE

24-341-0201

Inorganic Chemistry – II

(CHEMISTRY OF d- AND f-BLOCK ELEMENTS)

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: describe and explain the structure, bonding and magnetism in metal complexes using crystal field theory.	Analyse
C.O.2: describe various metal-ligand interactions in terms of sigma- and pi-bonding.	Analyse
C.O.3: identify various d-d transitions and interpret the electronic spectra of any given transition metal complex.	Evaluate
C.O.4: interpret the ESR spectra of any given transition metal complex.	Evaluate
C.O.5: explain the stability of metal complexes, their reactivity, and the mechanisms of ligand substitution and redox reactions.	Evaluate
C.O.6: interpret the Mossbauer spectra of iron complexes.	Apply

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	2	1	3	2	1
C.O.2	3	2	1	2	2	1
C.O.3	3	2	1	2	2	1
C.O.4	3	2	1	2	2	1
C.O.5	3	2	1	2	2	1
C.O.6	3	2	1	2	2	1

UNIT – 1 **(6 hrs)**

Crystal-field theory, d-orbital splitting in octahedral, tetrahedral, square planar, trigonal bipyramidal, trigonal planar and linear geometries, crystal field stabilization energy, effect of pairing energy.

Molecular Orbital Theory: construction of molecular orbital diagrams using group theory, qualitative MO diagrams for octahedral, tetrahedral and square planar complexes, effect of π-bonding, experimental evidence for π-bonding, spectrochemical series.

UNIT – 2 **(10 hrs)**

Microstates, Atomic term symbols, Free ion terms for dn configuration, Splitting of terms in octahedral and tetrahedral octahedral fields, Correlation diagram for d^2 configuration in octahedral geometry, d-d transitions, Selection rules for electronic transitions.

Orgel diagram – splittings for d^1, d^9, high spin d^4, d^6, splittings for high spin d^2, d^3, d^8 and d^7

Calculation of Dq, B and β

Tanabe Sugano diagrams – splittings for low spin d^n systems

Electronic Spectral interpretation of some coordination compounds

Consequence of Jahn Teller effect on the electronic spectra of coordination compounds

Charge transfer spectra, Electronic spectra of lanthanide and actinide complexes

UNIT – 3 **(6 hrs)**

Magnetism: brief review of different types of magnetic behaviours, spin-orbit coupling, quenching of orbital angular moments in crystal field, spin-only formula, correlation of μ_s and μ_{eff} values, magnetic moments of T terms and A, E terms, temperature independence paramagnetism, magnetic properties of lanthanides and actinides.

UNIT – 4 **(12 hrs)**

Electronic paramagnetic resonance spectroscopy: Electronic Zeeman effect, Zeeman Hamiltonian and EPR transition energy. Presentation of spectra. The effects of electron Zeeman, nuclear Zeeman and electron nuclear hyperfine terms in the Hamiltonian on the energy of the hydrogen atom. Second order effect. Hyperfine splittings in isotropic systems, spin polarization mechanism and McConnell's relations Anisotropy in g-value, EPR of triplet states, zero field splitting, Kramer's rule, survey of EPR spectra of first row transition metal ion complexes.

Mossbauer spectroscopy- Principles and applications to coordination compounds.

UNIT – 5 **(14 hrs)**

Reaction Mechanism: Thermodynamic and kinetic consideration, formation constant and rate constant, inert and labile complexes, factors affecting the stability and lability of complexes.

Ligand substitution in octahedral complexes, mechanism of substitution reactions in octahedral complexes, dissociative, associative and interchange mechanism, energy profile of reactions, acid and base hydrolysis, factors affecting the rate of substitution reactions in octahedral complexes.

Ligand substitution in square planar complexes, mechanism of substitution reactions in square planar complexes, energy profile of reactions, the trans effect and its applications, theories for explaining trans effect, factors affecting the rate of substitution reactions in square planar complexes.

Electron Transfer Reactions: inner sphere and outer sphere mechanism, Marcus theory, photochemical reactions

Recommended Text Books:

1. G.L. Miessler, P.J. Fischer, D.A. Tarr, Inorganic Chemistry, 5^{th} ed., Pearson, 2014.
2. F. A. Cotton, G. Wilkinson, C. A, Murillo, M. Bochmann Advanced Inorganic Chemistry, 6^{th} ed., Wiley-Interscience: New York, 1999.
3. J.E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of structure and Reactivity, 4^{th} ed., Harper Collin College Publishers, 1993.
4. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, 2^{nd} ed., John Wiley & Sons Ltd., 2009.

5. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd ed., ELBS, 1999.
6. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd ed., John Wiley and Sons, 1994.
7. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd ed., BH, 1997.
8. R. S.Drago, Physical Methods for Chemists, 2nd ed., Saunders College Publishing, 1992.
9. C. E. Housecroft, A. G. Sharpe, Inorganic Chemistry, 5th ed., Pearson, 2018.
10. W. L. Jolly, Modern Inorganic Chemistry, 2nd ed., McGraw-Hill, New York, 1991.
11. Leonard K. Nash, Elements of Chemical Thermodynamics, Addison Wesley, 2nd Edn, 2013.

CORE

24-341-0202

ORGANIC CHEMISTRY -II

(REACTIONS, REAGENTS AND SYNTHESIS)

Credit 4 **64 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Interpret the differences in reactivity of various reducing and oxidizing agents with mechanistic illustrations.	Apply
C.O.2: Analyse the reagents and conditions for the synthesis of specific target molecules.	Analyse
C.O.3: Describe strategies for the stereospecific/stereo selective organic transformations towards chiral target molecules.	Apply
C.O.4: Construct a synthetic pathway for simple to complex organic molecules by retrosynthetic approach.	Apply

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	2	1	3	3	1	1
C.O.2	2	1	3	3	2	1
C.O.3	1	1	3	3	2	1
C.O.4	1	1	3	3	2	1

UNIT – 1 **(12 hrs)**

Reagents for oxidation and reduction: Chromium reagents, activated DMSO, osmium tetroxide, selenium dioxide, singlet oxygen, peracids, hydrogen peroxide, periodic acid, lead tetraacetate, ozonolysis, Woodward and Prevost hydroxylation, Wacker process, Oppenauer oxidation, Sharpless, Shi and

Jacobsen asymmetric epoxidations. Catalytic hydrogenations (heterogeneous-Palladium/Platinum/Rhodium and Nickel, homogeneous-Wilkinson), metal hydride reduction- $LiAlH_4$, DIBAL-H, Red-Al, $NaBH_4$ and $NaCNBH_3$. Selectrides, trialkylsilanes and trialkyl stannane. Birch reduction, hydrazine and diimide reduction. Meerwein-Ponndorf-Verley reaction, Enzymatic reduction using Baker's yeast.

UNIT – 2 **(12 hrs)**

Synthetic applications of organometallic and organo-nonmetallic reagents: Hydorboration reactions, Sakurai allylation, Gilman's reagent, Ullmann and Glaser coupling reactions. Suzuki coupling, Sonogashira coupling, Heck reaction, Buchwald–Hartwig coupling, Negishi coupling and Stille coupling. Metathesis processes of electrophilic carbene complexes (first- and second-generation Grubbs catalyst), ROMP, Dötz reaction and methylenation of carbonyls.

Reagents such as NBS, DCC, DMAP, DEAD, DDQ. Phase transfer catalysts.

Chemistry of Nucleophilic Heterocyclic Carbenes (NHCs), multicomponent reactions such as Ugi reaction, Passerini reaction, Biginelli reaction. Click reaction.

UNIT – 3 **(12 hrs)**

Chemistry of carbonyl compounds: Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters, acyl halides and amides. Substitution at carbonyl carbon, mechanisms of ester hydrolysis, substitution at α-carbon, aldol and related reactions. Grignard reaction, Reformatsky reaction, Claisen, Darzen, Dieckmann, Knoevenagel and Stobbe condensations. Perkin, Prins, Mannich, Stork-enamine reactions. Conjugate additions, Michael additions and Robinson annulation. Favorskii reaction, Julia olefination, Peterson olefination.
Reaction with phosphorous and sulfur ylides.

UNIT – 4 **(14 hrs)**

Asymmetric Synthesis: Introduction to asymmetric synthesis, principle, general strategies, chiral pool strategy, chiral auxiliaries, chiral reagents – Binol derivatives of $LiAlH_4$, chiral catalysts – CBS catalyst. Stereospecific and stereoselective synthesis, determination of enantiomeric and diastereomeric excess.

Stereoselective nucleophilic additions to acyclic carbonyl groups-Cram's Rule, Felkin-Ahn Model, Effect of chelation on selectivity.

UNIT – 5 **(14 hrs)**

Synthesis planning and analysis: Convergent, divergent and parallel synthesis. Protecting groups- protection and deprotection of hydroxyl, carboxylic acids, carbonyls in aldehydes and ketones, amines, alkenes and alkynes. Chemo- & regioselective protection and deprotection. Functional group equivalents, reversal of reactivity (Umpolung). Disconnection approach-introduction to retrosynthesis, basic principles, synthons, and synthetic equivalents. Monofunctional and bifunctional disconnection, One group C-X and two group C-X disconnections, one group C-C and two group C-C disconnections. Retrosynthesis of longifoline, Corey lactone, Djerassi - Prelog lactone and D-luciferin.

Recommended Text Books:

1. M. B. Smith, Organic Synthesis, 2nd ed., McGraw-Hill, 2000.
2. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed., Wiley, 2013.
3. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.
4. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
5. P. S. Kalsi, Stereochemistry, Conformation and Mechanism, 9th ed., New Age Publications, 2017.

6. T. Tsuji, Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, John Wiley & Sons, 2000.
7. S. Warren, Organic Synthesis: The Disconnection Approach, 2nd ed., John Wiley, 2008.
8. E. Robert, Gawley, J. Aube, Principles of Asymmetric Synthesis, 2nd ed., Elsevier, 2012.
9. G. L. D. Krupadanam, Fundamentals of Asymmetric Synthesis, 1st ed., CRC press, 2014.
10. T.W. Greene, P. G. M. Wuts, Protecting Groups in Organic Synthesis, 2nd ed., John Wiley, 1991.
11. H. R. Crabtree, The Organometallic Chemistry of the Transition Metals, 6th ed., John Wiley & Sons, 2014.
12. S. D. Burke, R. L. Danheiser, Handbook of Reagents for Organic Synthesis, John Wiley & Sons, 1999.

CORE

24-341-0203

ORGANIC CHEMISTRY -III

(SPECTROSCOPY OF ORGANIC COMPOUNDS)

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Identify structures of unknown organic compounds using hyphenated techniques and spectral library matching.	Apply
C.O.2: Identify structures of unknown organic compounds based on the data from UV-Vis, IR, Mass Spectrometry ^{1}HNMR and ^{13}CNMR spectroscopy.	Apply

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	3	1	3	1	2
C.O.2	3	3	1	3	1	2

UNIT – 1 **(10 hrs)**

Study of Mass Spectrometry applied to organic molecular systems

Elemental analysis, empirical formula, molecular formula, Molecular mass, nominal mass, Exact mass, Index of hydrogen deficiency.

The technique of Mass Spectrometry: Molecular ion, ion production methods (EI). Soft ionization methods: FAB, CA, MALDI, PD, Field desorption electrospray ionization, HRMS and formula mass, LC-MS, GC-MS. MS- MS Mass spectra of chemical classes and its correlation with structure: Fragmentation patterns, nitrogen and ring rules, Rule of thirteen, McLafferty rearrangement.

UNIT – 2 **(10 hrs)**

Study of Ultraviolet-Visible Absorption and Emission and Chirooptical Spectroscopy applied to organic molecular systems

Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules, estimation of λmax of substituted aromatic ketones, aldehydes and acids. Spectral correlation with structure: Influence of substituents, conjugation, Intramolecular Charge transfer, Solvent effect

Fluorescence Spectroscopy. Excitation and Emission Spectra. Fluorescence Quantum Yield and Lifetime. Spectral correlation with structure: Influence of substituents, ring size, strain and conjugation, Intramolecular Charge transfer, Intramolecular proton transfer, Solvent effect

Chirooptical Spectroscopy: Introduction and applications of ORD, CD, Octant rule, axial haloketone rule, Cotton effect.

UNIT – 3 **(8 hrs)**

Study of Infrared Spectroscopy applied to organic molecular systems

Fundamental vibrations, overtones, Fermi Resonance, Hot bands, combination bands

Spectral correlation with structure: Characteristic regions of the spectrum. Influence of substituents, ring size, hydrogen bonding, vibrational coupling, hybridization and field effect on frequency.

IR spectra of chemical classes including amino acids and its correlation with structure

UNIT – 4 **(10 hrs)**

Study of NMR spectroscopy applied to organic molecular systems

The NMR instrumentation and Experiment: Magnetic nuclei with special reference to 1H and 13C nuclei. Chemical shift and shielding/deshielding, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. Proton and 13C NMR scales, characteristics of 13C as a nucleus.

Spin-spin splitting, AX, AX2, AX3, A2X3, AB, ABC, AMX type coupling, First order and non-first order spectra, Pascal's triangle, coupling constant, mechanism of coupling, Karplus curve, quadrupole broadening and decoupling, diastereomeric protons, virtual coupling, long range coupling effects, NOE, coupling with other nuclei.

Simplification non-first order spectra to first order spectra, shift reagents-mechanism of action, spin decoupling and double resonance, Chemical shifts and homonuclear/heteronuclear couplings, the basis of heteronuclear decoupling.

Polarization transfer. Selective Population Inversion (qualitative description only), DEPT, sensitivity enhancement and spectral editing. 2D NMR and COSY, HMQC, HMBC.

UNIT – 5 **(10 hrs)**

Identification of structures of unknown organic compounds using hyphenated techniques and Spectral library matching.

Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, Mass, 1HNMR and 13CNMR spectroscopy.

Recommended Text Books:

1. D. L. Pavia, G. M. Lampman, G. S. Kriz, J. R. Vyvyan, Introduction to Spectroscopy: A Guide for Students of Organic Chemistry, Indian ed., Brooks/Cole Cengage Learning, 2007.
2. Atta-Ur-Rahman, M. I. Choudhary, Solving Problems with NMR Specroscopy, Academic Press, New York, 1996.
3. L. D. Field; S. Sternhell, J. R. Kalman; Organic Structures from Spectra, 4th ed., Wiley 2008.
4. R. S. Drago, Physical Methods for Chemist, Saunders,1992.

5. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4^{th} ed., McGrawHill, 1994.
6. D. F. Taber, Organic Spectroscopic Structure Determination, A Problem Based Learning Approach, Oxford University Press, 2009.
7. R. M. Silverstein, G. C. Bassler, T. C. Morril, Spectroscopic Identification of Organic Compounds, John Wiley, 1991.
8. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw Hill, 1988.
9. W. Kemp, Organic Spectroscopy, 2^{nd} ed., ELBS-Macmillan, 1987.
10. F. Bernath, Spectra of Atoms and Molecules, 2^{nd} ed., Oxford University Press, 2005.
11. E. B. Wilson, Jr., J. C. Decius, P. C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Spectra, Dover Publications, 1980.
12. A. Weil, J. R. Bolton, Electron Paramagnetic Resonance: Elementary Theoryand Practical Applications, 2^{nd} ed., Wiley Interscience, John Wiley & Sons, Inc.,2007.
13. C. P. Slichter, Principles of Magnetic Resonance, 3^{rd} ed., Springer-Verlag, 1990.
14. H. Gunther, NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry, 3rd ed., Wiley- VCH, 2013.
15. Spectral data bases (RIO DB of AIST, for example).

CORE

24-341-0204

PHYSICAL CHEMISTRY- I

(STATISTICAL AND NON-EQUILIBRIUM THERMODYNAMICS)

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O. 1: Explain the different types of statistics and calculate the thermodynamic probability of any given thermodynamic system.	Analyse
C.O. 2: Calculate the partition function and thermodynamic properties from spectroscopic data.	Apply
C.O. 3: Apply the principles of statistical thermodynamics to ideal gases, solids and metals.	Apply
C.O. 4: Explain the basics of transport phenomena's viz., Osmosis, biological motors and electro kinetic effects.	Understand
C.O. 5: Derive expression for entropy production for physical and chemical processes	Apply

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	3	3	3	1	3
C.O.2	3	3	3	3	1	3
C.O.3	3	3	2	2	1	3
C.O.4	3	3	2	2	1	3
C.O.5	3	3	2	2	1	3

UNIT – 1 **(8 hrs)**

Kinetic Theory of gases, Maxwell Distribution of velocity, Boltzmann distribution, Types of molecular velocities- r.m.s, most probable and mean velocity, Molecular Collisions, Mean free path, Transport properties- Diffusion, effusion, Viscosity, Thermal conductivity.

Thermodynamic probability, microstate and macrostate, entropy andprobability, most probable distribution, residual entropy and its calculation. Ensembles, Maxwell - Boltzmann statistics.

UNIT – 2 **(10 hrs)**

Partition function and its relation to thermodynamic properties, Translational, rotational and Vibrational partition function. Molecular partition function for delocalized systems, calculation of equilibrium constant using partition functions. Heat capacity of gases, Anomalous heat capacity of H_2, Heat capacity of solids:

Dulong - Petits law, Einstein's theory and its modification, Debye's theory of heat capacity of solids.

UNIT – 3 **(10 hrs)**

Quantum statistics, Bose - Einstein statistics, Fermi - Dirac statistics, Comparison of Maxell - Boltzman, Bose=- Einstein and Fermi - Dirac Statistics, Dilute Systems. Application of Bose -Einstein Statistics, Gas degeneration, Application to liquid helium, Bose Einstein Condensation. Application of Fermi -Dirac Statistics to electrons in metals, Extreme Gas Degeneration, Electron gas in metals and its contribution to pressure and heat capacity.

UNIT – 4 **(10 hrs)**

Partition function for systems of dependent particles, Configurational integral and configurational partition function. Imperfect gas, van der Waals equation and Virial equation of state, Evaluation of the first virial coefficient. Condensed state, Cluster integrals, Communal entropy.

UNIT – 5 **(10 hrs)**

Linear Non-equilibrium thermodynamics- General theory, Local entropy production, balance equation for concentration. Energy conservation in open systems. Entropy balance equation. Forces and Fluxes, Steady state and local equilibrium conditions. Linear phenomenological laws. Phenomenological coefficient, Systems with heat, matter and electrical transport, Onsager Reciprocal relation, Application to Diffusion -Thermal diffusion, Thermal Osmosis and electrokinetic effects, Soret Coefficient, Seebeck effect.

Recommended Text Books:

1. F.W. Sears, Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics, Addision Wesley Pub. Cambridge, 1998.
2. F.C. Andrews, Equilibrium to Statistical Mechanics, John Wiley, New York, 2002.
3. L.K. Nash, Statistical Thermodynamics, Addison Wesley, New York, 1999.
4. P. W. Atkins, J. de Paula, Physical Chemistry 8th ed., 9th edn. Wiley, New York, 2006
5. D. A. McQuarrie, Physical Chemistry- A Molecular Approach, South Asian Edn., 2008.
6. M. Dole, Introduction to Statistical Thermodynamics, Prentice Hall, London, 1997.
7. J. Kestin, J.R. Dorfman, A Course in Statistical Thermodynamics, Academic press, 1971.
8. D. A. McQuarrie, Statistical Thermodynamics, South Asian Edn., 2008.
9. I. Prigogine, Introduction to Thermodynamic Irreversible Processes, 3rd ed.,Wiley Interscience, 1968.
10. S. R. de Groot, P. Mazur, Non-equilibrium Thermodynamics, Dover Publications, 2011.
11. G. Lebon, D. Jou, J. Casas, Understanding Non-equilibrium Thermodynamics, Springer. 2008.
12. S. Kjelstrup, D. Bedeaux, E. Johannessen, J. Gross, Non-Equilibrium Thermodynamics for Engineers: Second Edition, World Scientific Publishing Company, 2017.
13. D. Kondepudi and I. Prigogine, Modern Thermodynamics: From Heat Engines to dissipative Structures, Wiley, New York.

CORE

24-341-0205

THEORETICAL CHEMISTRY-III

(CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY)

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Account for the basic principles and concepts of molecular orbital theory and valence bond theory using quantum mechanical principles.	Understand
C.O.2: Explain Hartree-Fock Theory and semiempirical Huckel MO treatment and its application to polyelectronic molecules	Apply
C.O.3: .Classify various basis sets and justify its use for a specific problem	Apply
C.O.4: Explain different chemical properties of molecules by drawing molecular orbitals and analyze and interpret the results to solve chemical puzzles.	Evaluate

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	1	0	2	1	0
C.O.2	3	1	1	3	1	0
C.O.3	3	2	2	3	2	2
C.O.4	3	3	3	3	3	3

UNIT – 1 **(12 hrs)**

Chemical bonding, Born Oppenheimer approximation, Valence bond method. Comparison of VB and MO method, LCAO approximation, calculation of energy

levels from wave functions, application to diatomic molecules such as, H_2^+, H_2. Concept of σ, σ*, π, π* orbitals and their characteristics, hybrid orbitals, calculation of coefficients of AO used in sp, sp^2 and sp^3 hybrid orbitals, interpretation of geometry, Valence bond model of H_2, Hybridisation of H_2O,
BF_3, NH_3 and CH_4

UNIT – 2 **(8 hrs)**

Pi bonding in simple molecules, HMO method for linear conjugated hydrocarbons, linear, cyclic, polycyclic, heterocyclic; ethylene, 1,3-butadiene,allyl radical, cation and anion, aromatic hydrocarbons, cyclopropenyl systems, cyclobutadiene, benzene, naphthalene and other conjugated systems. calculation of charge distribution, bond orders and reactivity. QMOT: Applications of Molecular Orbital Theory in Understanding reactions and Mechanisms. Qualitative MO theory. Group orbitals. Frontier Orbitals, Substituent effects on frontier orbitals, HSAB concept, Nucleophiles and Electrophiles, Perturbation theory of reactivity. Application of Frontier Orbital theory in studying ionic and radical reactions, Ambident electrophiles, α-effect.

UNIT – 3 **(8 hrs)**

Tools and philosophy of computational chemistry. potential energy surface - local minima, global minima, saddle point and transition states, geometry optimization-stationary points.

UNIT – 4 **(8 hrs)**

Basis sets, Slater and Gaussian functions, classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, correlation consistent basis sets.

SCF methods, semiempirical, ab initio, electron correlations, post-Hartree-Fock methods and density functional theory.

UNIT – 5 **(12 hrs)**

Molecular structure, internal coordinates, Cartesian coordinates, geometry optimization, frequency analysis, partial charge, MO, Computational calculations listed below using available Molecular orbital theory suite of programme package: Constructing molecular structures or models; Molecular geometry optimization; Conformational analysis; Thermodynamic and spectroscopic properties; Molecular orbital analysis; Electron density and electrostatic potential map.

Recommended Text Books:

1. J. P. Lowe, Quantum Chemistry, 3rd ed., Academic Press, New York, 2008.
2. F. Jensen, Introduction to Computational Chemistry, 2nd ed., Wiley, New York, 2009.
3. R. Leach, Molecular Modeling, Principles and Applications, 2nd ed., Pearson Education, London, 2001.
4. A. K. Chandra, Introduction to Quantum Chemistry, 4th ed., Tata McGraw-Hill, 1994.
5. L. Pauling, E. B. Wilson, Introduction to Quantum Mechanics, McGraw-Hill, 1935.
6. A. Szabo, N. S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Book ed., Mc.Graw-Hill, New York, 1982.
7. T. A. Albright, J. K. Burdett, M.-H. Whangbo, Orbital Interactions in Chemistry, 2nd ed., John Wiley and Sons, Inc., Hoboken, New Jersey, 2013.

CORE/LAB

24-341-0206

ADVANCED PHYSICAL CHEMISTRY LAB

Credit 2 **64 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Operate various sophisticated instruments.	Apply
C.O.2: Perform experiments based on various laws of physical chemistry.	Apply
C.O.3: Analyse the results obtained from various experiments.	Analyse
C.O.4: Calculate the unknown concentration of the given solution based on the results obtained from the experiment.	Evaluate

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	3	3	3	2	3
C.O.2	3	3	3	3	2	3
C.O.3	3	3	3	3	1	3
C.O.4	3	3	3	3	2	3

UNIT – 1 **(64 hrs)**

i. Molecular weight determination by cryoscopic methods, Formula of complexes.

ii. Phase diagrams: Two component liquid–liquid and solid-liquid systems. Three component liquid-liquid systems.

iii. Determination of transition temperature, molecular weight determination.

iv. Refractometry: Variation of refractive index with composition, formula of complexes.

v. Chemical Kinetics: Acid and base catalysed hydrolysis of esters,

vi. Dependence of temperature and ionic strength on the rate of reactions, Hydrolysis of p-nitrophenyl acetate using spectrophotometry.

vii. Ostwald Viscometer: Viscosity of liquid and liquid mixtures.

viii. Conductometry: Cell constant, conductivity of a weak-acid, solubility of a sparingly soluble salt, conductometric titrations. Determination of critical micelle concentration of colloids.

ix. Potentiometry: Measurement of electrode potentials, activity coefficients and potentiometric titrations, pH metric titrations.

x. Adsorption: Checking the validity of Freundlich and Langmuir adsorption and determination of unknown concentration.

xi. Spectrophotometry: Checking the validity of beer Lambert's law and determination of unknown concentration.

xii. Demonstration of instrumentation of AAS, Flame photometry, Fluorescence spectrometer, GPC, Electrochemical work station etc.

Recommended Text Books:

6. A. Findlay, Practical Physical Chemistry, 9th ed., Longman, 1973.
7. D. P. Shoemaker, C.W. Garland, J.W, Nibler, Experiments in Physical Chemistry, 5th ed., McGraw Hill, 1989.
8. J. B. Yadav, Advanced Practical Physical Chemistry, 36th ed., Krishna Prakashan Media (P) Ltd, 2016.
9. J. N. Gurtu, A.N. Gurtu, Advanced Physical Chemistry Experiments, 6th ed., Pragati, 2014.

CORE/LAB

24-341-0207

OPEN ENDED LAB-I

Credit 2 **32 Hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Design experiments and validate the hypothesis of an independent research problem.	Evaluate

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	2	2	3	3	2	3

UNIT – 1

The students shall perform literature review/ experiments/analysis for validating the hypothesis and submit Research Progress Report.

ELECTIVE

24-341-0208

BIOANALYTICAL CHEMISTRY

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Demonstrate key features and characteristics of major biomolecules.	Understand
C.O.2: Describe and explain the principles and applications of MRI and NMR for bioanalysis.	Understand
C.O.3: Outline the principles and theory of major types of electrophoresis and electrophoretic separation.	Apply
C.O.4: Explain the theory and applications of biochemical analysis like RIA, ELISA.	Analyze
C.O.5: Appreciate the variety of popular methods to separate and isolate biomolecules.	Evaluate

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	3	0	1	3	1
C.O.2	3	3	2	1	3	1
C.O.3	3	3	3	2	3	1
C.O.4	3	3	3	2	3	1
C.O.5	3	3	2	2	3	1

UNIT – 1 **(10 hrs)**

Biomolecules- amino acid, protein, nucleic acid –structures, physical and chemical properties, features and characteristics of major biomolecules, structure-function relationship, significance. Different methods for the estimation of protein. Transition metals in health and disease - Importance of transition metals in physiological processes, Therapeutic implications of transition metals.

UNIT – 2 **(10 hrs)**

Transmission electron Microscopy (TEM), Scanning electron Microscopy (SEM) – Instrumentation and its biological applications. Nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) technologies: key tools for the life and health sciences. Principles of NMR and the importance of this biomolecular analytical technique. Established and emerging applications of NMR.

Principles and uses of MRI. MRI as a principal diagnostic and research tool.

UNIT – 3 **(10 hrs)**

Electrophoretic techniques – Principles of electrophoretic separation. Types of electrophoresis including paper, gel. Electrophoresis, Pulse field gel electrophoresis- applications in life and health science.

UNIT – 4 **(10 hrs)**

Radio immune assay (RIA) - principle and applications. Enzyme linked immune sorbent assay (ELISA) principle and applications. Biosensors-applications.

UNIT – 5 **(8 hrs)**

Principle of centrifugation, concept of RCF, features and component of major types of centrifuge, preparative, differential and density gradient centrifugation, analytical ultra-centrifugation, centrifugation. Flow cytometry: principles and applications of this core method of separation.

Recommended Text Books:

1. V. A. Gault, N. H. Mcclenaghan, Understanding bio analytical chemistry - principle and applications, John Wiley and Sons, Ltd Publications, 2009.
2. A. Manz, N. Pamme, D. Iossifidis, Bio-analytical Chemistry, 2004
3. S. R. Mikkelsen, E. Corton, Bio Analytical Chemistry, John Wiley and Sons, Ltd Publications, 2004.
4. K. Wilson, J. Walker, Practical Biochemistry-Principles and techniques, 5th ed., Cambridge University press, 2000.

ELECTIVE

24-341-0209

ADVANCED PHOTOCHEMISTRY

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Describe various photochemical and photophysical processes and apply established experimental methods for the investigation of these processes.	Apply
C.O.2: Explain theories of photoinduced energy and electron transfer and their significance in different fields including biomedical applications, and artificial light harvesting system.	Evaluate
C.O.3: Apply the knowledge of photochemistry of semiconductors and advanced materials for various applications involving photochemical energy conversions.	Apply

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	3	2	2	2	3
C.O.2	3	3	1	2	2	3
C.O.3	3	3	2	2	2	3

UNIT – 1 **(14 hrs)**

Introduction to Photochemistry: Light Matter Interactions, Importance and Time Scale of Photoinduced Processes, Emission Spectrum, Excitation Spectrum, Characteristics: Stoke's Shift, Kasha's Rule, Mirror Image Rule, Fluorescence and Phosphorescence, Lifetime, Quantum Yields, Mechanisms of Spectral Shift, Solvatochromism, Lippert-Mataga Equation, Photochromism, Excimers, Exciplexes

UNIT – 2 **(10 hrs)**

Instrumentation-Fluorescence Spectrometer, Quantum Yield Measurements, Lifetime Measurement, Light Sources, Monochromators, Optical Filters, Detectors, Polarizers, Ideal Spectrometers, Distortion and Corrections in Measurements, Inner Filter Effects

UNIT – 3 **(12 hrs)**

Fluorescence Quenching, Theories of Static Quenching and Dynamic Quenching, Derivation of Stern-Volmer Equation, Deviations, Energy and Electron Transfer Basic Concepts- Donor-Acceptor Systems, Photoinduced Energy Transfer – Trivial Mechanism, Dexter Mechanism, Forster Mechanism, Efficiency, Distance Measurements, Photoinduced Electron Transfer- Libby's Theory, Marcus Theory

UNIT – 4 **(12 hrs)**

Applications of Photoinduced Process: Singlet Oxygen – Methods of Singlet oxygen generation and Detection – Chemistry of Singlet Oxygen – Photodynamic Therapy of Cancer, Fluorescence Sensors, Artificial Light-Harvesting Systems, Photosynthesis, Photocatalysis, Photochemical Water Splitting. Atmospheric Photochemistry, Dye Sensitized Solar Cells - Bulk Heterojunction Solar Cells, Luminescent Solar Concentrator, Organic Light Emitting Devices. Photoresists – Photolithography – Photochromism – Photonic Materials and Lasers.

Recommended Text Books:

1. N. J. Turro, V. Ramamurthy, J. C. Scaiano, Modern Molecular Photochemistry of Organic Molecules, University Science Books, 2010.
2. C.E. Wayne, Photochemistry (Oxford Chemistry Primers), Oxford University Press; 1st ed., 1996.
3. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, Plenum Press, 3rd ed., 2010.
4. A. M. Braun, M.-T. Maurette, Esther Oliveros, Photochemical Technology, John Wiley & Sons, 1991.
5. M. A. Fox, M. Chanon, Photoinduced Electron Transfer Part A, B. C and D, Elsevier Science Publishing Company, 1988.
6. J. Mattay Ed., Photoinduced Electron Transfer 1-5 (Topics in Current Chemistry), Springer, 1st ed., 1990-1993.

7. G. J. Kavarnos, Fundamentals of Photoinduced Electron Transfer, 1st ed., Wiley-VCH, 1993.
8. V. Ramamurthy, K. Schanze, Molecular and Supramolecular Photochemistry, Volume 10, Semiconductor Photochemistry and Photophysics, Marcel Dekker, New York, 2003.
9. V. Ramamurthy, Photochemistry in Organized and Confined Media, VCH Publishers, NewYork,1991.

ELECTIVE

24-341-0210

THEORY OF ORBITAL INTERACTIONS IN CHEMISTRY

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Examine the physical properties associated with molecules and the pathways taken by chemical reactions.	Analyse
C.O.2: Correlate qualitatively the shape and energy of orbitals and the chemical reaction exhibited by any molecule.	Apply
C.O.3: Explore the effects of symmetry, overlap, and electronegativity in the molecular orbital in case of chemical reaction.	Evaluate
C.O. 4: Explore the structures and reactivity relationships associated with any molecule.	Evaluate

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	1	0	3	1	0
C.O.2	3	1	1	2	1	0
C.O.3	3	2	1	2	1	1
C.O.4	3	3	2	2	2	2

UNIT – 1 **(8 hrs)**

Atomic and Molecular Orbitals, Concepts of Bonding and Orbital Interaction, Orbital Interaction Energy, Molecular Orbital Coefficients, Electron Density Distribution, Perturbational Molecular Orbital Theory, Linear H_3, HF, and the Three-Orbital Problem.

UNIT – 2 **(10 hrs)**

Molecular Orbital Construction from Fragment Orbitals, Triangular H_3, Rectangular and Square Planar H_4, Tetrahedral and Linear H_4, Pentagonal H_5 and Hexagonal H_6, Molecular Orbitals of Diatomic Molecules and Electronegativity Perturbation, Geometrical Perturbation of Molecular orbitals, Molecular Orbitals of AH_2, Walsh Diagrams, Jahn–Teller Distortions.

UNIT – 3 **(10 hrs)**

Molecular Orbitals of Small Building Blocks, AH System, AH_3 Systems, pi-Bonding Effects of Ligands, AH_4 System, Molecules with Two Heavy Atoms, A_2H_6 Systems, Orbital Interactions through Space and through Bonds.

UNIT – 4 **(8 hrs)**

Polyenes and Conjugated Systems, Acyclic Polyenes, Huckel Theory, Cyclic Systems, Conjugation in Three Dimensions, Solids, Energy Bands, Hypervalent Molecules.

UNIT – 5 **(12 hrs)**

Transition Metal Complexes. Octahedral ML_6, pi-Effects in an Octahedron, Distortions from an Octahedral Geometry, Square Planar, Tetrahedral ML_4 Complexes, Five Coordination, Square Pyramidal ML_5 Fragment, ML_3 Fragment, ML_2 and ML_4 Fragments, M_2L_8 Dimers, CpM and Cp_2M, Isolobal Analogy.

Recommended Text Books:

1. T. A. Albright, J. K. Burdett, M.-H. Whangbo, Orbital Interactions in Chemistry, 2nd ed., John Wiley and Sons, Inc., Hoboken, New Jersey, 2013.
2. I. Flemming, Molecular Orbitals and Organic Chemical Reactions, Students ed., Wiley, 2009.
3. A. Rauk, Orbital Interaction Theory of Organic Chemistry, 2nd ed., Wiley-Blackwell, 2000.
4. W. L. Jorgensen, L. Salem, The Organic Chemist's Book of Orbitals, Academic Press, 1973. .

ELECTIVE

24-341-0211

TRANSITION METALS: CHEMISTRY AND APPLICATIONS IN ORGANIC SYNTHESIS

Credit 3 **48 hours**

Course outcome After the completion of the course, the student will be able to	**Cognitive level**
C.O.1: Describe the structure, bonding and properties of transition metal complexes	Understand
C.O.2: Predict and explain the principle and mechanism involved in transition metal-mediated transformations	Apply
C.O.3: Construct organic molecules for various applications using palladium reagents	Apply
C.O.4: Predict the structure and reactions of various metal-carbene complexes	Apply
C.O.5: Apply transition metal complexes for various asymmetric transformations	Apply

	Programme Specific Outcomes					
Course outcomes	**P.S.O.1**	**P.S.O.2**	**P.S.O.3**	**P.S.O.4**	**P.S.O.5**	**P.S.O.6**
C.O.1:	2	1	2	2	1	1
C.O.2:	3	1	2	3	1	2
C.O.3:	1	1	3	3	1	2
C.O.4:	3	1	3	3	1	2
C.O.5:	1	1	3	3	1	2

Unit - 1 **(10 hrs)**

Basic concepts in organometallic chemistry: Introduction, 18 electron rule and its limitations, electron counting with examples, oxidation state, types of ligands, bonding, back-bonding. Formation of transition metal complexes, coordination number and geometry. σ-Bonded and π-bonded organometallic compounds.

Unit - 2 (**12 hrs)**

Mechanisms involved in transition metal chemistry:

Oxidative addition, reductive elimination, transmetallation, migrative insertion, β-hydride elimination, nucleophilic and electrophilic attack on transition metal complexes. C-H activation. Catalytic mechanism of hydrogenation and hydroformylation. Single electron transfer and radical reactions. Homogeneous and heterogeneous catalysis.

Unit - 3 **(12 hrs)**

Reactions mediated by palladium-based reagents:

Characteristics of organopalladium compounds, catalysts and precursors, mechanistic features of cross- coupling reactions, reactivity of substrates, selectivity. Palladium catalysed coupling reactions: Corriu-Kumada reaction, Hiyama reaction, Suzuki coupling, Sonogashira coupling, Heck reaction, Buchwald–Hartwig coupling, Negishi coupling, Stille coupling. Miscellaneous reactions catalysed by palladium- Direct arylation, cyanation, carbonylation, Tsuji-Trost allylic substitution, α-allylic alkylation and α-fluorination.

Unit - 4 **(10 hrs)**

Transition metal carbene complexes:

Structure and properties. Fischer carbene complexes-preparation and reactions. Schrock carbene complexes-preparation and reactions. Non-stabilised carbene complexes. Metathesis process of carbene complexes.

Unit – 5 **(10 hrs)**

Transition metals in asymmetric catalysis:

Asymmetric catalysis in metathesis, epoxidation, allylation, hydroformylation, isomerisation of allylic amines, hydrocyanation, hydrogenation, Heck reaction and Pauson–Khand reaction.

Recommended Text Books:

1. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 6th Edn., John Wiley & Sons, 2014.
2. L. S. Hegedus, B. C. G. Soderberg, Transition Metal in the Synthesis of Complex Organic Molecules, 3rd Edn., University of Science Books, 2010.
3. D. Astruc, Organometallic Chemistry and Catalysis, Springer, 2007.
4. J. Tsuji, Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, John Wiley & Sons, 2002.
5. I. Omae, Applications of Organometallic Compounds, John Wiley & Sons, 1998
6. R. Bates, Organic Synthesis Using Transition Metals, 2nd Edn., John Wiley & Sons, 2012.
7. B. Gabriele, Organic Synthesis *via* Transition Metal-Catalysis, MDPI, 2022.
8. K. Grela, Olefin Metathesis, John Wiley & Sons, 2014.

ELECTIVE

24-341-0212

NEW METHODS AND STRATEGIES IN ORGANIC SYNTHESIS AND DYNAMIC STEREOCHEMISTRY

Credit 4 **Hours 64**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O. 1: To learn various organic reactions and reagents used in them as tools applied in the art of organic synthesis.	Apply
C.O. 2 : Analyze the reagents and conditions for the synthesis of specific target molecules.	Analyze
C.O. 3: To learn and apply various concepts such as stereochemistry and fundamental principles of stereoselectivity in organic chemistry.	Apply
C.O. 4: Analyze the effect of molecular conformation in the outcome of a reaction	Analyze

	Programme Outcomes									
Course Outcomes	P.O. 1	P.O. 2	P.O. 3	P.O. 4	P.O. 5	P.O. 6	P.O. 7	P.O. 8	P.O. 9	P.O. 10
C.O.1	X	X						X		
C.O.2	X		X					X		
C.O.3	X		X					X		
C.O.4	X		X					X		

UNITI **14hrs**

Chemo-, regio- and stereoselective functional groups interconversions; oxidation and reduction processes and their synthetic utility; metal-free oxidation (boron-, peroxide-, sulfur-, iodine-based) and metal-based (Ru-, Cr-, Mn-, Os-, Pd-) reagents; transfer hydrogenation; enantioselective oxidation and reduction processes.

UNIT II **12hrs**

Strategic carbon-carbon and carbon-heteroatom bonds formation; carbon-carbon multiple bonds construction processes and corresponding named reactions; functional group transposition; conjunctive reagents;
construction of cyclic frameworks; fused and spirocyclic systems.

UNIT III **12hrs**

Domino/Cascade reactions: principles and advantages; rationalization with examples of radical, anionic, cationic, and pericyclic domino/cascade processes.

UNIT IV **13hrs**

Stereoselectivity in cyclic molecules: Introduction; Stereochemical control in six-membered rings; Reactions on small rings; Regiochemical control in cyclohexene epoxides; Stereoselectivity in bicyclic compounds; Fused bicyclic compounds; Spirocyclic compounds; Reactions with cyclic intermediates or cyclic transition states.

UNIT V **13hrs**

Diastereoselectivity: Prochirality; Diastereoselective additions to carbonyl groups without rings; Stereoselective reactions of acyclic alkenes; Stereoselective Aldol reactions; Single enantiomers from diastereoselective reactions.

Recommended Text Books:

1. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1996
2. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier Academic Press, 2005
3. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009
4. J. Clayden, N. Greeves, and S. Warren, Organic Chemistry, Oxford University Press, 2nd Edition, 2012
5. L. F. Tietze, G. Brasche, and K. Gericke, Domino Reactions in Organic Synthesis, Wiley, 2006
6. Roderick Bates, Organic Synthesis using Transition Metals, 2nd Edition, Wiley, 2012

7. George S. Zweifel and Michael H. Nantz, Modern Organic Synthesis: An Introduction, W. H. Freeman Publisher, 2007.
8. P.S.Kalsi: Stereochemistry, Conformation and Mechanism, 3rd edn., New Age Publications
9. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, Pearson Education, New Delhi.
10. Bruckner, R. Advanced Organic Chemistry: Reaction Mechanisms, 1st edn., Academic Press, 2001.

ELECTIVE

24-341-0213
MATERIAL CHEMISTRY

3 credits **48 hrs**

CO	CO Statement	CL	PSO
CO1	To acquire basic knowledge on various types of materials	Understand	1,3, 4,5,6
CO2	To gain insight on the structure – property relationship of different materials.	Understand	1,3, 4,5,6
CO3	To get knowledge on various characterization techniques.	Analyze	1,3, 4,5,6
CO4	To get an idea about the materials in advanced technological applications	Apply	1,3, 4,5,6

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	0	1	3	2	2
CO2	3	0	1	3	2	2
CO3	3	0	1	3	3	2
CO4	3	0	1	3	3	2

Unit I **(8 hrs)**

Chemistry of Materials. Ionic and covalent solids. Molecular and metallic solids.

Amorphous and crystalline materials. Crystalline state. Structural organization

of crystalline solids-theories of bonding. Crystal structures. Imperfections in crystal structures.

Semiconductor materials- properties and types of semiconductors. Structure and Bonding of semiconductor materials. Silicon based semiconductors. II-VI (wide band gap) and III-V (narrow band gap) compound semiconductors. Electrical, optical and magnetic properties of semiconductor materials. Preparation and properties of ZnO, ZnS, CdS, CdTe, Ga-As, In-S, Cu-In-S. Application in photovoltaic devices.

Unit II **(10 hrs)**

Polymer Materials- classification and nomenclature of polymers. Methods of Polymerization. Structure–property relationships. Plastics and elastomers. Viscoelastic behaviour. Rubber like elasticity. Crystalline and amorphous polymers. Glass transition temperature and crystalline melting. Functional Polymers.

Unit III **(10 hrs)**

Nanomaterials. Materials in the nanodomain. Zero, one- and two-dimensional materials. Particle size dependent change in properties of materials. Metals in the nanodomain. Gold and silver nanoparticles. Preparation, properties and applications.

Core shell structures. Semiconductor nanoparticles. Quantum dots. ZnO, ZnS, CdS and CdSe quantum dots.

Electrical and optical properties. Nano domains of Carbon-fullerenes, carbon nanostructures, graphene, graphene quantum dots.

Unit IV **(10 hrs)**

Characterization of Materials. Optical Microscopy- Principles, instrumentation and application of confocal Raman microscopy, SPM/STM. Electron microscopy- SEM, FESEM, TEM. Principles, instrumentation and applications. Surface and core level techniques- Photoelectron spectroscopy - X-Ray and UV. Thermal methods- TG/DTG, DTA, DSC, DMA. X-Ray Diffraction.

Unit V **(10 hrs)**

Materials in Advanced Technology. Organic Polymer Semiconductors, Solid ionic conductors -Advanced materials for energy generation and energy storage.

Porous membranes. Optical and photonic materials.

Recommended Books:

1. B. D. Fahlman, Materials Chemistry, 2nd ed. Springer, Heidelberg, 2011.
2. Harry R. Allcock, Introduction to Material Chemistry, John Wiley & Sons, Inc., New Jersy, 2008
3. R. Zallen, Physics of Amorphous Solids, Wiley, New York, 1983.
4. R. J. Borg, G. J. Dienes, The Physical Chemistry of Solids, Academic Press, Boston, 1993.
5. D. Kingery, H. K. Bowen, D. R. Uhlmann, Introduction to Ceramics, 2nd ed., Wiley, New York, 1992.
6. J. M. J. Cowie, Polymers. Physics and Chemistry of Modern Materials, 3rd ed., CRC Press, Boca Raton, 2007.
7. S. O. Kasap, Principles of Electronic Materials and Devices, Mc Graw Hill, 2006

Semester 2

CORE

24-341-0301

ADVANCED ANALYTICAL CHEMISTRY AND INSTRUMENTAL METHODS

Credit 4 **64 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O. 1: Explain the theory, instrumentation and applications of various electroanalytical techniques, chromatographic, thermal and surface analysis	Apply
C.O.2: Predict appropriate chromatographic methodology for separation of a given mixture	Analyse
C.O.3 : Perform individual and simultaneous voltammetric analysis of samples	Evaluate
C.O. 4 : Analyse the surface of various samples using SEM, AFM, TEM	Analyse

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	2	3	3	3	2	2
C.O.2	2	3	3	3	2	2
C.O.3	2	3	3	3	2	2
C.O.4	2	3	3	3	2	2

UNIT – 1 **(18 hrs)**

Potentiometry: different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, biomembrane, biological and biocatalytic electrodes as biosensors, importance of selectivity coefficients. CHEMFETS- importance of specially designed amplifier systems for ion selective electrode systems. Potentiometric titrations- types and applications.Electrogravimetry- electrogravimetry without potential control, controlled potential electrogravimetry, applications

Coulometry- constant current and constant potential coulometry, applications- primary and secondary coulometry, advantages of coulometric titrations

Conductance measurement – conductometric titrations

Polarography – current – voltage curve, DME-components of polarographic current, supporting electrolyte, polarographic maxima. Half-wave potential, Applications of Polarography

Voltammetry - different types, Theory and applications

Stripping analysis. Amperometric titrations – Different types and Applications

Impedance spectroscopy, Voltammetric sensors – individual and simultaneous analysis-Case study

UNIT – 2 **(12 hrs)**

Gas chromatography – basic instrumental set up-inlets, carriers, columns, detectors and comparative study of TCD, FID, ECD, NPD and MS. Qualitative and quantitative studies using GC, Preparation of GC columns, packet columns and capillary columns, selection of stationary phases of GLC, Choosing theparameters- Temperature, Length of the column, Sample size, Flow rate

CHN analysis by GC, Case study

GC Capillary electrophoresis-migration rates and plate heights, instrumentation, sample introduction, detection methods, applications. Capillary gelelectrophoresis. Capillary isotachophoresis. Isoelectric focusing.

Capillary electro chromatography-packed columns. Micellar electro kinetic chromatography and GC-MS applications

UNIT – 3 **(12 hrs)**

HPLC – Separation process, Eddy diffusion, Mass transfer, Longitudinal diffusion, Retention parameters in HPLC-Capacity factor, Retention time, Retention volume, Peak width, Total number of theoretical plates, Height equivalent of a theoretical plate, Resolution and retention time, Solvent delivery systems, Detectors Instrumentation and functioning of HPLC, Types of HPLC - Modes of separation in HPLC-adsorption chromatography, reversed phase chromatography, ion pair chromatography, ion exchange chromatography Solubility and retention in HPLC Method development in HPLC - Selection of mobile phase and optimization, Preparation of sample, Selection of column and solvent

HPLC method validation, HPLC Analysis -Case study Dos and Don’ts in HPLC - Troubleshooting in HPLC

UNIT – 4 **(12 hrs)**

Measurement of alpha, beta, and gamma radiations, neutron activation analysis and its applications. Principle and applications of isotope dilution methods, Radioimmunoassay (RIA), Immunoradiometric assay (IRMA), Enzyme linked immunosorbent assay (ELISA)-Principles and practical aspects

Thermal methods of Analysis TG, DTA and DSC - Instrumentation and Theory – Factors affecting TGA - effect of atmosphere on DTA. TG of copper sulphate pentahydrate and calcium oxalate monohydrate. Application of thermal methods for identification of substances.

UNIT – 5 **(10 hrs)**

Chemical Analysis of surfaces: Surface preparations-ion scattering spectrometrysecondary ion scattering microscopy (SIMS)-Auger election spectroscopy-ESCA instrumentation and application.

Principle, instrumentation and applications of SEM, TEM and AFM, Case study

Recommended Text Books:

1. J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.
2. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
3. J.G. Dick, Analytical Chemistry, R.E. Krieger Pub., 1978.
4. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
5. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's Text Book of Quantitative Chemical Analysis, 5th Edn., John Wiley& sons,1989.
6. C.L. Wilson, D.W. Wilson, Comprehensive Analytical Chemistry, Elsevier, 1982.
7. G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.
8. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.
9. H.A. Laitinen, W.E. Harris, Chemical Analysis, McGraw Hill, 1975.
10. F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, Blackwell Science, 2000.
11. Contemporary Instrumental Analysis, Kenneth A. Rubinson, Judith F. Rubinson, Prentice Hall, New Jersey, 2000.
12. Wilson & Wilson's, Comprehensive Analytical Chemistry, Volume 47, Modern Instrumental Analysis, Edited by S. Ahuja, N. Jespersen, Reed Elsevier India Private Ltd., Noida, 2006.
13. Journal of Chromatography Library, Volume 3, Liquid Column Chromatography-A Survey of Modern Techniques and Applications, Edited by Z. Deyl, K. Macek, J. Janak, Elsevier Scientific Publishing Company, Amsterdam, 1975.
14. Gas Chromatography, John Willett, John Wiley & Sons, Singapore, 1991.
15. Fundamentals of Analytical Chemistry, Doughlas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Ed., Cengage Learning, 2014.
16. Allen J. Bard, Larry R. Faulkner, Electrochemical Methods-Fundamentals and Applications, JohnWiley & Sons, NewYork, 1980.

CORE

24-341-0302

Inorganic Chemistry – III

(ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY)

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: distinguish the different types of ligands with respect to the type of interaction with the metal.	Analyse
C.O. 2: evaluate the structure, bonding and reactions of organometallic compounds and metal clusters.	Evaluate
C.O.3: predict the stability of organometallic compounds and metal clusters.	Apply
C.O.4: explain the application of reactions of organometallic complexes in homogeneous catalytic processes.	Apply
C.O.5: identify the role of metals in biological systems.	Apply

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	1	0	3	1	0
C.O.2	3	1	0	3	1	0
C.O.3	3	1	0	3	1	0
C.O.4	3	1	0	3	1	1
C.O.5	3	1	0	3	1	0

UNIT – 1 **(8 hrs)**

Compounds with transition metal to carbon bonds: eighteen electron rule; classification of ligands, nomenclature, σ donor ligands – metal alkyl, aryl complexes; σ donor/π acceptor ligands, – metal alkenyls, alkynyls, carbenes, carbynes, carbonyls, isocyanide, fluxionality of ligands – structure, bonding, spectra, preparation and reactions.

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UNIT – 2 **(8 hrs)**

σ, π donor/π acceptor ligands – olefin complexes, alkyne, allyl, enyl complexes, metallocene- ferrocene, titanocene, zircanocene, arene complexes, cycloheptatriene, cyclooctatetraene, cyclobutadiene complexes, fluxionality of ligands – structure, bonding, preparation, reactions and spectroscopy

UNIT – 3 **(8 hrs)**

Metal–Metal bonds and Transition metal clusters; preparation, properties and spectroscopy. Parallels with nonmetal chemistry - isolobal analogy.Application of Wade – Mingos - Lauher rules in predicting the structure of organometallic clusters

UNIT – 4 **(12 hrs)**

Reactions of organometallic complexes – Ligand cone angle, oxidative addition, reductive elimination, insertion, nucleophilic and electrophilic attack of coordinated ligands. Homogeneous catalysis using organometallic compounds: olefin hydrogenation, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, olefin isomerisation, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation, coupling reactions in organic chemistry

UNIT – 5 **(12 hrs)**

Metal ions in biological systems: Heme proteins – hemoglobin, myoglobin Non-Heme Iron Proteins: Iron storage and transfer – ferritin, transferrin; electron transfer (Iron-sulfur protein) – rubredoxin, ferredoxin; O2 transport – hemerythrin Copper proteins and Enzymes –Hemocyanin, superoxide dismutase, ceruloplasmin, cytochrome co-oxidase;

Zinc and Cobalt enzymes – carbonic anhydrase, carboxypeptidase, interchangeability of zinc and cobalt enzymes; Vitamin B12 and B12 Photosynthesis and N2 fixation Metals in medicines and therapy

Recommended Text Books:

1. Ch. Elschenbroich, A. Salzer, Organometallics – A Concise Introduction, VCH Publishers, 1989.
2. B. D. Gupta, A. J. Elias, "Basic Organometallic Chemistry", University Press, 2010.
3. P. Powell, Principles of Organometallic Chemistry, 2nd ed., ELBS, 1991.
4. J. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.
5. E.-I. Ochiai. Bioinorganic Chemistry – An Introduction, Allyn and Bacon Inc., 1977.
6. N. Kaim, B. Schwederski. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley, 1994.
7. Bertini, H. B. Gray, S. J. Lippard, J. S. Valentine, Bioinorganic Chemistry, Viva Books, 1998.
8. R. W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987.
9. J. A. Cowan, Inorganic Biochemistry – An Introduction, 2nd ed., VCH, 1997.
10. N. S. Hosmane (Ed) Boron Science: New Technologies and Applications, CRC Press, 2011.
11. S. J. Lippard, J. M. Berg. Principles of Bioorganic Chemistry, Panima Publ. Corpn. 2005.
12. M. N. Hughes, The Inorganic Chemistry of Biological Processes, Wiley, 1981.

CORE

24-341-0303

ORGANIC CHEMISTRY-IV

(CHEMISTRY OF NATURAL PRODUCTS)

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Device synthesis scheme for nonaromatic organic heterocyclic aromatic and compounds.	Analyse
C.O.2: Elucidate structure and device synthesis for important natural products.	Apply
C.O.3: Describe molecular structure of carbohydrates, proteins, DNA, RNA and synthesis of vitamin C and shikimic acid.	Understand

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	1	1	3	3	2	1
C.O.2	1	2	3	3	3	2
C.O.3	1	1	3	2	2	0

UNIT – 1 **(8 hrs)**

Nomenclature and general characteristics of heterocyclic compounds. Structure, properties, synthesis and reactivity of three and four-membered ring heterocycles containing one heteroatom.

UNIT – 2 **(12 hrs)**

Heteroaromatic compounds (five and six-membered rings) containing one or two heteroatoms. Fused ring compounds: Synthesis and properties of indole, quinoline, isoquinoline, coumarin, flavone, purine and pyrimidine bases present in nucleosides.

UNIT – 3 **(10 hrs)**

Terpenoids: Classification, biosynthesis. Structure elucidation and synthesis of abietic acid. Steroids: classification, biosynthesis. Structure elucidation of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone. Fatty acids: structure, biosynthesis. Prostaglandins-classification, structure, biosynthesis and synthesis.

Alkaloids: Classification, isolation, structure elucidation based on degradative reactions (quinine and atropine). Biosynthesis of quinine and papaverine.

UNIT – 4 **(10 hrs)**

Carbohydrates: Structure of ribose, glucose, fructose, maltose, sucrose, lactose, starch cellulose and cyclodextrins. Preparation of alditols, glycosides (O, C, and N), deoxysugars. Synthesis of Vitamin C from glucose. Nucleic acids: Structure and synthesis, genetic code, recombinant DNA, biosynthesis of shikimic acid.

UNIT – 5 **(8 hrs)**

Amino acids, peptides and enzymes: Synthesis of amino acids – Strecker and azalactone synthesis, enantioselective synthesis of amino acids, reactions of amino acids. Structure of proteins, introduction to enzymes and coenzymes with special reference to the function of chymotrypsin, NAD, thiamine, pyridoxal. In vitro and in vivo synthesis of peptides, solid phase synthesis.

Recommended Text Books:

1. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.
2. I. L. Finar, Organic Chemistry Volumes 1 & 2, 6th ed., Pearson Education Asia, 2004.
3. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.

4. N. R. Krishnaswamy, Chemistry of Natural Products; A Unified Approach, Universities Press, 1999.
5. R. J. Simmonds, Chemistry of Biomolecules: An Introduction, RSC, 1992.
6. R. O. C. Norman, Principles of Organic Synthesis, 2nd ed., Chapman and Hall, 1978.
7. J. A. Joule, K. Mills, Heterocyclic Chemistry, 5th ed., Wiley, 1998.
8. J. J. Li, E. J. Corey, Total Synthesis of Natural Products: At the Frontiers of Organic Chemistry, Springer, 2012.
9. T. Eicher, S. Hauptmann, The Chemistry of Heterocycles, 2nd ed., Wiley, 2003.
10. K. C. Nicolaou, S. A. Snyder, Classics in Total Synthesis II: More Targets, Strategies, Methods, Wiley,2003.

CORE

24-341- 0304

PHYSICAL CHEMISTRY-II

(CHEMICAL KINETICS, REACTION DYNAMICS, CATALYSIS AND SURFACE CHEMISTRY)

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O. 1: Interpret the basic reaction dynamics and obtain the rate constants for reactions in gaseous state and solutions.	Analyse
C.O. 2: Calculate thermodynamic parameters from kinetic data.	Apply
C.O. 3: Interpret the kinetics of unimolecular, termolecular and fast reactions.	Apply
C.O. 4: Identify isotope effects in reactions	Analyse
C.O. 5: Apply the principles of acid-base and enzyme catalysis to solve any given kinetic data.	Analyse

	Programme Specific Outcomes					
Course Outcomes	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O.1	3	3	3		1	
C.O.2	3		3		1	
C.O.3	3		3		1	
C.O.4	3	3	3		1	
C.O.5	3	3	3		2	

UNIT – 1 **(8 hrs)**

Complex Reactions- Parallel, Consecutive and Opposing reactions, Steady state Approximation, Kinetics of chain reactions - Photochemical reactions H_2-Cl_2 and H_2-Br_2 reaction, Organic decomposition reactions-Rice Herzfield mechanism (acetaldehyde and ethane), Branched Chain Reactions, Explosions-

Semenov Hinshelwood mechanism (H_2-O_2 reaction),

Fast Reactions- Relaxation methods- Perturbations, Flash photolysis and Pulse radiolysis

UNIT – 2 **(10 hrs)**

Molecular reaction dynamics: Reactive encounters, Theories of reaction rates- Collision Theory. Collision and reaction cross section. Activated Complex Theory- PES, Erying equation, Comparative evaluation of collision and transition state theory, Thermodynamic treatment of reaction rates. Theory of unimolecular reactions- Lindemann Mechanism, Modifications to Lindemann mechanism- Hinshelwood, RRK and RRKM model. Termolecular reactions. Molecular beam methods, Stripping and rebound mechanism

UNIT – 3 **(10 hrs)**

Reactions in Solutions – Cage effect, Transition state theory for reactions in solutions, Effect of ionic strength, dielectric constant and Internal pressure. Primary and secondary salt effect. Solute-solvent interactions. Ion dipole and dipole-dipole reactions. Diffusion controlled reactions.

Isotope effects: Equilibrium isotope effects. Primary and Secondary kinetic isotope effects.

UNIT – 4 **(10 hrs)**

Surfaces and interfaces: Surface free energy and Surface tension, Contact angles and Wetting, Surface films. capillarity, vapour pressure of droplets- Kelvin equation. pressure difference across curved surface -Laplace equation, Surface wetting- hydrophilicity and hydrophobicity.

Physical and chemical adsorption. Adsorption isotherms- Langmuir (kinetic and statistical derivation), Freundlich and BET (derivation) isotherms, Determination of surface area using Langmuir and BET isotherms, Isosteric heat of adsorption. Thermodynamics of adsorption- Gibbs adsorption isotherm.

UNIT – 5 **(10 hrs)**

Catalysis and Inhibition, heterogeneous Catalysis – Transition state theory, General mechanism. General Mechanism of homogeneous catalysis- Arrhenius and vant Hoff intermediates, Acid base catalysis- specific and general acid catalysis, Enzyme catalysis- Michaelis-Menten Mechanism, Competitive and non competitive inhibition. Unimolecular and bimolecular Surface reactions- Kinetics of adsorption- Langmuir Hinshelwood mechanism and Rideal-Eley mechanism.

Autocatalysis- Oscillatory reactions- Lotka- Volterra, Oregonator, Brussellator.

Recommended Text Books:

1. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, New York.
2. K. J. Laidler, Chemical-Kinetics, McGraw Hill, New York.
3. M. R. Wright, An Introduction to Chemical Kinetics, Wiley, 2004.
4. Richard Masel, Chemical kinetics and Catalysis, Wiley Interscience.
5. P. W. Atkins, Physical Chemistry 8th Edn., Wiley, New York.
6. Christian Reichardt, Solvents and Solvent effects in Organic Chemistry, Wiley VCH 2003.
7. A. W. Adamson, The Physical Chemistry of Surfaces, 2nd Edn., Wiley. New York.
8. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, New York.
9. K. J. Laidler, Chemical-Kinetics, McGraw Hill, New York.
10. M. R. Wright, An Introduction to Chemical Kinetics, Wiley, 2004.
11. A. Somorjai, Chemistry of Surfaces, 3rd Edn. Wiley, New York.
12. Clark, "Theory of adsorption and catalysis", Academic Press, 1970.
13. J.M. Thomas & W.J. Thomas, "Introduction to principles of heterogeneous catalysis", Academic Press, New York, 1967.
14. R.H.P. Gasser, "An introduction to chemisorption and catalysis by metals", Oxford, 1985.
15. D.K Chakraborthy, "Adsorption and catalysis by solids", Wiley Eastern Ltd. 1990.

CORE

24-341-0305

PHYSICAL CHEMISTRY-III

ADVANCED ELECTROCHEMISTRY

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: describe the theories effecting ionic conductance and apply the concepts to calculate conductance behaviour of a given system.	Apply
C.O.2: describe the electronic conductance behaviour in charged interfaces and analyse the catalytic behaviour of a system.	Analyse
C.O.3: learn the working principle and advancement in futuristic electrochemical devices.	Understand

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	3	3	2	2	1
C.O.2	3	3	3	2	1	1
C.O.3	3	3	3	1	1	1

UNIT – 1 **(8 hrs)**

Review of basic concepts, Ionic Conductance, Ion Solvent Interactions, Ion-Water Interactions, Coordination Number, Solvation numbers, Hydration of simple cation, anion, and transition metal ion. Ion-Ion Interaction, Debye-HuckelTheory, Ionic Atmosphere, time of Relaxation, Mechanism of Electrolytic Conductance, Linearized P-B equation, Activity and Activity Coefficient of Electrolytes, Validity of Deby-Huckel theory., Debye-Hückel limiting law,
Debye-Hückel-Bronsted Equation.

UNIT – 2 **(12 hrs)**

Ion transport, Fick's law of diffusion, Diffusion Coefficient, Ionic drift in presence of electric field, drift velocity, transport number, Debye-Huckel-Onsager Equation, Relaxation effect, time of relaxation, Determination of degree of dissociation, Debye-Falkenhagen Effect, Wien Effect.

Ionic liquids, Limiting case of zero solvent-pure electrolyte, features of ionic liquid, diffusion in IL, ionic conductance IL, liquid oxide electrolytes.

UNIT – 3 **(12 hrs)**

Electrodics, Charged Interfaces, Electrode Potential, Factors Influencing electrode potential, Band Bending, electrolytic polarization, dissolution and decomposition potential, concentration polarization. Concentration cells.

Structure of electrified interfaces, liquid junction potential, the electrode double layer, electrode-electrolyte interface, different models of double layer, theory of multilayer capacity, electrocapillary, Lippmann equation, membrane potential

UNIT – 4 **(8 hrs)**

Electrode kinetics, Ion adsorption, Electron Transfer Under an Interfacial Electric Field, Overvoltage, theories of overvoltage, Tafel equation, Butler-Volmer equation. Electrocatalyst- Homogeneous, heterogeneous, Randles-Sevcik Equations, Pourbiax diagrams, PCET.

UNIT – 5 **(8 hrs)**

Semiconductor electrode interface. Band bending, photoelectrochemistry, fuel cells, battery-metal –ion, metal-air battery, Corrosion, Bioelectrochemistry – nervous system, enzyme as electrodes.

Recommended Text Books:

1. J. Bockris, A. K. N. Reddy, Modern Electrochemistry-1 Ionics, 2nd ed., Springer Science & Business Media, 2018.
2. J. Bockris, A. K. N. Reddy, M. E. Gamboa-Aldeco, Modern Electrochemistry-2A: Fundamentals of Electrodics, 2nd ed., Springer Science & Business Media, 2018.
3. J. Bockris, A. K. N. Reddy, Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology and Environmental Science, 2nd ed., Springer Science & Business Media, 2018.
4. R. Crow, Principles and Applications of Electrochemistry, 4th ed., 1994.
5. S. Glasstone, An Introduction to Electrochemistry, Paperback ed., 2007.

24-341-0306
SPECTROSCOPIC TECHNIQUES

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Explain the fundamentals of spectroscopy.	Understand
C.O.2: Correlate the structure of molecule with UV-Visible and IR spectral data.	Apply
C.O.3: Interpret first order NMR spectra.	Analyse
C.O.4: Determine the primary structure of peptides based on mass spectra.	Analyse
C.O.5: Examine secondary structure of peptides based on IR, NMR and mass spectral data.	Evaluate
C.O. 6: Explain the applications of X ray and microscopic techniques.	Understand

	Programme Specific Outcomes					
Course Outcomes	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O.1	3	3	1	3	3	1
C.O.2	3	3	2	2	3	2
C.O.3	3	3	2	3	3	2
C.O.4	3	3	2	2	3	2
C.O.5	3	3	2	2	3	2
C.O.6	3	3	2	2	3	2

INTERDEPARTMENTAL ELECTIVE

UNIT – 1 **(8 hrs)**

Different regions of electromagnetic spectrum and energy associated with a particular frequency, Types of spectroscopic techniques, Energy levels in molecules. Population of energy levels, basics of light absorption, factors affecting sensitivity, intensity and width of spectral lines, absorption characteristics, structural information based on absorption characteristics

UNIT – 2 **(10 hrs)**

UV-visible spectroscopy – Principle, allowed and forbidden transitions, chromophores, auxochromes, effect of structure on absorption characteristics

Basics of ORD and CD and emission spectroscopy.

IR spectroscopy –Principle, intra and intermolecular hydrogen bonding, effect of concentration and temperature, Fourier transform IR, group frequencies, fundamental frequencies, overtones, Fermi Resonance.

UNIT – 3 **(10 hrs)**

Experimental aspects of FT NMR, factors influencing sensitivity and resolution, Proton NMR, Chemical shift, Applications of chemical shift, spin-spin coupling, Analysis of spin systems, factors affecting coupling constants, NMR of Carbon-13, DEPT analysis and brief introduction to correlation spectroscopy (COSY, HMBC and HSQC). Brief introduction to NMR of other biologically relevant nuclei such as ^{15}N, ^{2}D and ^{31}P.

UNIT – 4 **(12 hrs)**

Mass spectrometry - high resolution mass spectrometry, soft ionization techniques, MS/MS data, application of GC-MS and LC-MS data, introduction to fragmentation modes and determination of primary structure of peptides on the basis of mass spectral data.

Problems based on combined application of various spectroscopic techniques to examine secondary structure of peptides.

INTERDEPARTMENTAL ELECTIVE

UNIT – 5 **(14 hrs)**

Introduction to microscopic and X-ray techniques. Confocal microscopy, fluorescence and radioisotope labeling as diagnostic tools. Basic introduction to Electron microscopy: types, sample preparation and analysis. Powder XRD and single crystal XRD

Recommended Text Books:

1. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, A Guide for Students of Organic Chemistry, 3rd ed., Thomson. 2004.
2. Atta-Ur-Rahman, M. I. Choudhary, Solving Problems with NMR Specroscopy, Academic Press, New York, 1996.
3. L. D. Field, S. Sternhell, J. R. Kalman, Organic Structures from Spectra, 4th ed., Wiley, 2008.
4. R. S. Drago, Physical Methods for Chemist, Saunders, 1992.
5. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th ed., McGrawHill, 1994.
6. D. F. Taber, Organic Spectroscopic Structure Determination, A Problem Based Learning Approach, Oxford University Press, 2009.
7. H. Gunther, NMR Spectroscopy, 2nd ed., John Wiley and Sons, 1995.
8. R. M. Silverstein, G. C. Bassler, T. C. Morril, Spectroscopic identification of organic compounds, John Wiley, 1991.
9. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw Hill. 1988. 10. W. Kemp, Organic Spectroscopy, 2nd ed., ELBS-Macmillan, 1987.
10. F. Bernath, Spectra of Atoms and Molecules, 2nd ed., Oxford University Press, 2005.
11. E. B. Wilson, Jr., J. C. Decius, P. C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Spectra, Dover Publications, 1980.
12. A. Weil, J. R. Bolton, Electron Paramagnetic Resonance: Elementary Theoryand Practical Applications, 2nd ed., Wiley Inter Science, John Wiley & Sons, Inc., 2007.
13. C. P. Slichter, Principles of Magnetic Resonance, 3rd ed., Springer-Verlag, 1990.
14. H. Gunther, NMR Sprectroscopy: Basic principles, Concepts, and Applications in Chemistry, 2nd ed., Wiley 1997.
15. Spectral data bases (RIO DB of AIST, for example).

INTERDEPARTMENTAL ELECTIVE

24-341-0307

INTRODUCTION TO MOLECULAR MODELING IN CHEMISTRY

Credit 3 **48 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O. 1: Appreciate the evolution of quantum mechanics and correlate the concepts to modern electronic structure.	Apply
C.O. 2: Differentiate the various methods to understand the electronic structure and apply it rationally.	Analyze
C.O. 3: Construct the structure of polyatomic molecule in terms of internal coordinates.	Apply
C.O. 4: Use computational chemistry softwares to perform and interpret various computations.	Analyse

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	1	0	3	1	0
C.O.2	3	2	2	3	2	2
C.O.3	2	1	1	2	1	1
C.O.4	3	3	3	3	3	3

UNIT – 1 **(10 hrs)**

The Schrödinger Equation, The Time-Independent Schrödinger Equation, BornOppenheimer approximation, The Molecular Potential Energy Surface, Multiple Minima, Saddle Points, Characterization, Finding Minima, LCAO, Hartree-Fock theory, Roothan–Hall equations, Koopmans theorem, HF limit and electron correlation.

INTERDEPARTMENTAL ELECTIVE

UNIT – 2 **(10 hrs)**

Basis sets, basis set approximation, Slater and Gaussian functions, contractions, polarization and diffuse functions, split-valence sets, classification of basis sets – minimal, double zeta, triple zeta, correlation-consistent sets, core-valence sets, general contractions, EMSL basis set exchange.

UNIT – 3 **(10 hrs)**

Semi empirical methods, post Hartree-Fock Method, Configuration interaction, Manybody perturbation theory, Coupled-cluster theory, Nondynamical correlation and multiconfigurational self-consistent-field (MCSCF) theory, Density Functional Theory, Hybrid QM/MM.

UNIT – 4 **(8 hrs)**

Input of molecular structure, Z-matrix construction, single point energy calculations, geometry optimizations, Electronic Energy, Vibrational frequency analysis, symmetry analysis, zero-point vibrational energies (ZPVE's), distinguishing minima from transition states, Intrinsic reaction coordinate (IRC) analysis, transition barrier and activation energy, conformational energetics, reaction energetics, enthalpy of formation, bond dissociation energy, ionization energy, isomerization energy and barrier, potential energy surface, reaction mechanism, enthalpy, entropy and free energy changes for reactions, isodesmic reactions.

UNIT – 5 **(10 hrs)**

Introduction to molecular mechanics; The Force Field Energy, The stretch energy, The bending energy, The out-of-plane bending energy, The torsional energy, The van der Waals energy, The electrostatic energy: charges and dipoles, Force Field Parameterization, Universal force fields, Advantages and Limitations of Force Field Methods, Basics of Molecular Dynamics Simulation, Generating and Analyzing a Molecular Dynamics Trajectory, Methods for Calculation of Free Energy, Application to Intermolecular Interactions and Binding Energies, Solvation Models, Combined QM/MM methods, Application of QM/MM to Enzyme.

INTERDEPARTMENTAL ELECTIVE

Recommended Text Books:

1. C. J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2^{nd} ed., John Wiley & Sons, 2004.
2. F. Jensen, Introduction to Computational Chemistry, 3^{rd} ed., Wiley, New York, 2017.
3. A. R. Leach, Molecular Modelling Principles and Applications, 2^{nd} ed., Pearson Education Limited, 2001
4. I. N. Levine, Quantum Chemistry, 7^{th} ed., Pearson, 2013.

INTERDEPARTMENTAL ELECTIVE

24-341-0308

ADVANCED TECHNIQUES IN ORGANIC SYNTHESIS: THEORY AND PRACTICE

Credit 3 **48 Hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Independently organizing and carrying out the most sophisticated and widely used organic transformations in a safe lab setting.	Apply
C.O.2: Characterize simple to complex molecules using spectroscopic methods.	Apply

	Programme Specific Outcomes					
Course Outcomes	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O.1	3	3	3	3	3	1
C.O.2	3	3	3	3	3	1

UNIT-1 **(9 hrs)**

General methods in organic synthesis: Condensation, substitution, cycloaddition, oxidation, and reduction. Methods for heterocycles and their important reactions**.**

UNIT-2 **(9 hrs)**

Advanced organic reactions: Multicomponent reactions, organo-catalysed reactions, click reactions. Cross-coupling reactions, metathesis reactions, and application in the synthesis of functional molecules and drugs.

UNIT-3 **(24 hrs)**

Practice : General methods of separation and purification of organic compounds such as 1) solvent extraction 2) thin layer chromatography and paper chromatography 3) column chromatography.

INTERDEPARTMENTAL ELECTIVE

Drawing the structures of organic molecules and reaction schemes by Proprietary and open source computer software. Use Chemical Abstracts, Scopus, Scifinder etc., to search, analyse and collect chemical information.

UNIT-4 **(24 hrs)**

Practice: Hands-on training in conducting reactions under an inert atmosphere and usage of Schlenk line techniques. Drying of solvents like THF, methanol and toluene. Handling of the Glove box. Green strategies such as microwave, sonochemistry, electrochemical and photochemical reactions. Training in cross-coupling reactions and olefin metathesis.

UNIT-5 **(24 hrs)**

Practice: Characterization of synthesized molecules using GC, LCMS, IR, NMR and HPLC techniques. Determination of specific rotation of enantiopure molecules.

Recommended Text Books

1. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
2. A. I. Vogel, A. R. Tatchell, B. S. Furnis, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, 5th ed., John Wiley, 1989.
3. P. S. Kalsi, Stereochemistry, Conformation and Mechanism, 10th ed., New Age Publications, 2019.
4. T. Tsuji, Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, John Wiley & Sons, 2000.
5. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, A Guide for Students of Organic Chemistry, 3rd ed., Thomson. 2004.
6. J. R. Mohrig, D. G. Alberg, G. E. Hofmeister, P. F. Schatz, C. N. Hammond, Laboratory Techniques in Organic Chemistry, 4th ed., W. H. Freeman and Company, 2014.

CORE/LAB

24-341-0401
PROJEC DISSERTATION

Course Outcome After the completion of the course the student will be able to	**Cognitive level**
C.O.1: Identify and hypothesise an advanced level research problem.	Create
C.O.2: Design experiments and validate the hypothesis of an advanced level research problem.	Create

	Programme Specific Outcomes					
Course Outcomes	**P.S.O. 1**	**P.S.O. 2**	**P.S.O. 3**	**P.S.O. 4**	**P.S.O. 5**	**P.S.O. 6**
C.O.1	3	3	3	3	3	3
C.O.2	3	3	3	3	3	3

UNIT – 1

The students shall carry out research project in reputed research laboratory for the entire semester.

The students shall submit a project report on the research work carried out.

The students will have to present the results of the research project in a seminar and appear for a comprehensive viva-voce.

Guide lines for setting up Question Papers in Theory Courses

1. The entire syllabus must be covered in the question paper.
2. Each question must be mapped to a specific C.O.
3. All the C.O.s must be reflected in the question paper.
4. The question paper may consist of questions at different cognitive levels such that, 20% of “remember” level, 40% of “understand” level and 40% of “apply and higher” level.

END