Post Graduate Syllabus in Chemistry
For
Four Semester M.Sc. Course (2 Years)
Under
Choice Based Credit System (CBCS)
(Revised on 14.12.2018)

Department of Chemistry

DIBRUGARH UNIVERSITY

Dibrugarh-786004

Assam, India

Department of Chemistry: Dibrugarh University

M.Sc Syllabus in Chemistry under Choice Based Credit System (CBCS) (Revised on 14.12.2018)

1. Name of Course: M.Sc (Chemistry) – Four Semester System

Structure of the syllabus

	Semester I		
Course	Course title	Credit	Marks (End Semester+Internal Assessment)
Core 101	Inorganic Chemistry-I	4	100 (60+40)
Core102	Organic Chemistry-I	4	100 (60+40)
Core103	Physical Chemistry-I	4	100 (60+40)
DSE 104 A or DSE 104 B	Laboratory Course-I Laboratory Course-II	6 6	150 (90+60) 150 (90+60)
AEC105	Analytical Chemistry-I	2	50 (30+20)
	Total	**20**	**500**

	Semester II		
Course	Course title	Credit	Marks (End Semester+Internal Assessment)
Core 201	Inorganic Chemistry-II	4	100 (60+40)
Core 202	Organic Chemistry-II	4	100 (60+40)
Core 203	Physical Chemistry-II	4	100 (60+40)
DSE 204 A or DSE 204 B	Laboratory Course-III Laboratory Course-IV	6 6	150 (90+60) 150 (90+60)
GE 205	Materials Chemistry	4	100 (60+40)
	Total	**22**	**550**

	Semester III		
Course	Course title	Credit	Marks (End Semester+Internal Assessment)
Core 301	Inorganic Chemistry-III	4	100 (60+40)
Core 302	Organic Chemistry-III	4	100 (60+40)
Core 303	Physical Chemistry-III	4	100 (60+40)
DSE 304 A or DSE 304 B	Laboratory Course-V Laboratory Course-VI	6 6	150 (90+60) 150 (90+60)
GE 305	Green and Sustainable Chemistry	4	100 (60+40)
AEC 306	Analytical Chemistry-II	2	50 (30+20)
	Total	**24**	**600**

<u>In Semester IV, a student has to select any one of the following tables. Course Core 407 will be common to all students.</u>

	Semester IV **(Inorganic Chemistry Specialization)**		
Course	Course title	Credit	Marks (End Semester+Internal Assessment)
Core401	Inorganic Chemistry-IV	4	100 (60+40)
Core402	Inorganic Chemistry-V	4	100 (60+40)
Core 407	General Approaches to Research	4	100 (60+40)
DSE 408	Project	8	200 (120+80) (Dissertation=90; Viva-voce=30)
	Total	**20**	**500**

	Semester IV (Organic Chemistry Specialization)		
Course	Course title	Credit	Marks (End Semester+Internal Assessment)
Core 403	Organic Chemistry-IV	4	100 (60+40)
Core 404	Organic Chemistry-V	4	100 (60+40)
Core 407	General Approaches to Research	4	100 (60+40)
DSE 408	Project	8	200 (120+80) (Dissertation=90; Viva-voce=30)
	Total	**20**	**500**

	Semester IV (Physical Chemistry Specialization)		
Course	Course title	Credit	Marks (End Semester+Internal Assessment)
Core 405	Physical Chemistry-IV	4	100 (60+40)
Core 406	Physical Chemistry-V	4	100 (60+40)
Core 407	General Approaches to Research	4	100 (60+40)
DSE 408	Project	8	200 (120+80) (Dissertation=90; Viva-voce=30)
	Total	**20**	**500**

Total Credit = 86

Total Marks = 2150

SEMESTER I

Course: Core 101 (Inorganic Chemistry-I)

Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To gain basic knowledge about structures and bonding of simple inorganic molecules.
2. To gain insight into acid base concept in Inorganic Chemistry
3. To provide a broad foundation in inorganic biochemistry

Expected Learner Outcome:

1. Students will learn the importance of structural and bonding nature of inorganic molecules.
2. Students will develop concepts on acid base chemistry from the inorganic chemistry perspective.
3. Student will gather knowledge about role of different metals and nonmetals in biological system.

Unit I: Chemical Bonding **Lecture 20, Marks 25**

VSEPR Theory: Structure of molecules containing lone pair(s) of electrons, structure andhybridization, Bent's rule, Bent bond, Non-bonded repulsion and structure.

LCAO-MO methods in homo and heteronuclear diatomic molecules (O_2, N_2, CO, NO).MOdescription of tri and tetraatomic molecules (CO_2, NO_2, NO_2^+, CO_3^{2-}, O_3 and NO_3^-).

Bonding in electron deficient compounds. Structure and bonding in boranes, carboranes,metallocarboranes, S-N and Se-N and P-N compounds.

Metallic and Metal ligand bonding: Spinel and Perovskite structures. Ionic surrounding: Crystal Field Theory; Covalent surrounding : Transition metal MO and ligand field Theory, Transition metal complexes with σ and π bonding ligands. Molecular orbital model, General view of ML_6 and ML_4 structures: ML_6(Oh), ML_4(D4h) and ML_4(Td).

Chemical periodicity, Chemical hardness, Application of electronegativity.

Unit II: Acid Base and Redox Chemistry **Lecture 13, Marks15**

Acid-Base concepts, Measure of Acid-Base Strengths, Acid-Base in water.Non-aqueoussolvent, aprotic solvent and superacids. Hard and Soft Acids and Bases, application of SHAB

principle.

Half cell reaction, reduction potential, application of reduction potential data, electrochemical series; brief idea of corrosion and its prevention; Nernst equation. Latimer and Frost diagram (V, Mn Fe, Cu etc.),disproportionation reaction; cyclic voltametry.

Unit III: Bioinorganic Chemistry **Lecture 17, Marks 20**

Fundamentals of inorganic biochemistry, essential, non-essential and role of 3d block elements and non-metals in bio-systems.

Natural and synthetic oxygen carriers,Porphyrins, model compounds for oxygen binding and carriers: Hemoglobin, myoglobin, hemerythrin, hemocyanin, Electron transfer protein:

Cytochromes, Iron-Sulphur, Nitrogen fixation. Metalloenzymes, corrinoids (vitamin B12 and co-enzyme), carboxy-peptidases, chlorophyll and photosynthesis, Na-K or ATPase or sodium pump, crown ethers, futuristic aspects of organo-transition metal complexes in bioinorganic chemistry.

Text Books:

1. Bioinorganic Chemistry by K. Hussain Reddy, New Age International Publisher.

Recommended Books:

1. The Inorganic Chemistry of Biological Processes, Hughes, M.N., 2nd edition, Wiley (1981)
2. Bio-coordination Chemistry, D.E. Fenton, Oxford University Monograph Series 1995.
3. Inorganic Chemistry, Gary L.Miessler & Donald A. Tarr 3rd Ed, Pearson
4. Inorganic Chemistry, C.E. Housecraft & A.G. Sharpe, 2nd Ed, Pearson

Course: Core 102 (Organic Chemistry-I)
Credit 4
Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To provide students the fundamental knowledge on structure, reactivity and reaction mechanism of organic compounds.
2. To design organic transformations through disconnection approach.
3. Application of spectroscopic techniques for compound characterization

Expected Learner Outcome:

1. Students will gain an insight to the various types of bonding and their implications in reactivity and properties of organic compound.
2. Students will acquire expertise in designing newer synthetic methodologies through disconnection approach and characterization of the products using spectroscopic techniques.

Unit I **Lecture 10, Marks12**

Structure, bonding and reactivity of organic compounds :Aromaticity, antiaromacity and homoaromaticity, metallocenes, tropolones and azulenes.
Supramolecularchenmistry: Bonds weaker than covalent bond – charge transfer complexes, inclusion complexes and crown ethers. Cryptand, rotaxanes,
Fullerenes, Graphenes. Phase transfer catalyst.
Hammet equation, Taft equation. Influence of reaction medium on rates.

Unit II **Lecture 10, Marks12**

Organic reaction mechanism – Transition state vs. Reaction intermediate, Energy profile of multistep reaction, Significance of rate limiting step in multistep reactions, Catalysed and uncatalysed reactions, Kinetic vs. Thermodynamic control, Kinetic and non-kinetic methods of studying organic reaction mechanism; Isotope labeling studies and kinetic isotope effects, Cross-over experiment. Reactivity - selectivity principle :Chemoselectivity, regioselectivity, stereoselectivity and stereospecificity in substitution, elimination and addition reactions. Neighbouring group effects.
Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes.

Unit III **Lecture 10, Marks12**

Stereochemistry: Concept of prostereoisomerism and prochirality – Homotopic and heterotopic ligands and faces; Optical purity and enantiomeric excess; Chirality in molecules devoid of chiral centers - allenes, spirans and biphenyls. Classification of stereoselective synthesis: diastereoselective and enantioselective reactions; Stereo-differentiating approach, Nucleophilic addition to aldehydes and acyclic ketones: Cram and Felkin – Ahn model. Enantioselective synthesis – Use of chiral reagent, chiral catalyst and chiral auxillary.Resolution – optical and kinetic.

Unit IV **Lecture 10, Marks12**

Disconnection approach in organic synthesis: Acceptor and donor synthons, Use of umpolung, Retrosynthesis of Alcohols (Grignard approaches and hydride transfer approaches) and Carbonyl compounds. One group and two group C-X disconnections. One group and two group C-C disconnections. Retrosynthsis of 1,2-, 1,3-, 1,4-, 1,5- and 1,6-difunctional (O,O and N,O in a difunctional relation) compounds.

Use of protecting groups in organic synthesis: protection and deprotection of hydroxyl, dihydroxy, carbonyl, carboxyl and amino groups.

Unit V **Lecture 10, Marks12**

NMR spectroscopy: Chemical shift, factors affecting chemical shift, spin- spin interaction, Coupling constant and Factors affecting, relaxation processes, NOE, Nuclear magnetic double resonance, shift resonance, spin tickling; Proton and ^{13}C NMR spectroscopy of simple organic molecules, living systems – MRI, : Two dimensional NMR, NOESY, DEPT, INEPT terminology, Instrumentation, FT NMR.

IR:Application of IR in organic spectroscopy

Text Books:

1. Organic Chemistry, Vols I and II – I. L. Finar, ELBS.
2. Stereochemistry and Mechanism through Solved Problems- P.S. Kalsi, New Age International Publishers
3. Introduction to Spectroscopy – by Donald L. Pavia, Cengage Learning India Private Limited
4. A Guidebook to Mechanism in Organic Chemistry– Peter Sykes, Longman, New York.

Recommended Books:

1. Organic Chemistry – R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Prentice Hall India Limited
2. Organic Chemistry – Paula Yurkanis Bruice, Pearson
3. Advanced Organic Chemistry: Reaction Mechanism and Structure – Jerry March, Wiley Eastern.
4. Stereochemistry of Organic Compounds – D. Nasipuri, Wiley Eastern
5. Stereochemistry of Carbon Compounds – Earnest E. Eliel, Tata McGraw Hill
6. Stereochemistry of Carbon Compounds – Subrata Sengupta, New Central Book agency, Kolkata
7. Disconnection Approach in Organic Synthesis – S. Warren, Wiley
8. Organic Reaction Mechanism, Christine Willis and martin Willis, Oxford chemistry Primers (No. 74)
9. Disconnection Approach in Organic Synthesis – S. Warren, Wiley
10. Designing Organic Synthesis – S. Warren, Wiley, Chichester
11. The Logic of Organic Synthesis – E.J. Corey and Xue Min Chen, Wiley, New York

Course: Core 103 (Physical Chemistry-I)
Credit 4
Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To impart knowledge on the concepts fugacity, activity, partial molar quantities and third law of thermodynamics.
2. To understand the fundamental ideas and basic principles of quantum mechanics and its applications to simple model systems.
3. To impart the foundations of rotational, vibrational and electronic spectroscopies with the help of Quantum Chemical model systems.

Expected Learner Outcome:

1. Students will understand the fundamentals and develop skills to solve problems related to fugacity, activity, partial molar quantities and third law of thermodynamics.
2. Students will be motivated to develop perception of matter from Quantum Mechanical viewpoint.
3. Students will know and understand the basic principles of Quantum Chemistry.
4. Students will gain the knowledge of fundamentals of spectroscopy and its analysis. They will also develop skills to apply these knowledge to solve problems in spectroscopy.

Unit I: Equilibrium thermodynamics **Lecture 10, Marks 15**

Concept of fugacity and it determination. Ideal solution and non ideal solutions, Activity and activity coefficient, Determination of activity coefficient, excess function for non-ideal solutions.

Partial molar quantities: chemical potential, Determination of partial molar volume, Thermodynamics of mixing.

Third law of thermodynamics, its experimental verification, determination of absolute entropy.

Unit II: Quantum Chemistry-I **Lecture 16, Marks 15**

Review of the basic principles of Quantum Mechanics: Postulates, Linear and Hermitian operators, commutation relation, related important theorems.

Model Systems: Free particle and particle in a box (One and three dimensional), degeneracy. Simple Harmonic Oscillator-Schrodinger equation and its solution, Hermite polynomials, two-particle rigid rotor- rotational energy levels of diatomic molecules, particle in a ring, quantum mechanical tunnelling.

Unit III: **Spectroscopy** **Lecture 24, Marks 30**

Electromagnetic spectrum, Interaction of emr with matter, Natural line width and Broadening- Intensity of spectral transitions.Selection rules.

Rotational (microwave) spectroscopy: Classification of molecules according to their moments of inertia, rotational energy levels of HCl, Selection rule for Microwave spectra, intensity, effect of substitution in Microwave spectra. Stark effect, spectra of symmetric top and asymmetric top type molecules.
Fundamental vibrational frequencies, Selection rules and vibrational energy for harmonic and anharmonic oscillators, vibration rotational spectra of diatomic molecules, Fundamental, overtone and combination bands, P, Q and R branches, hot bands, group frequencies, normal modes of vibrations, symmetry of vibrations.
Quantum theory of Raman effect, Selection rules, mutual exclusion principle, vibration-rotation Raman spectra. Intensity of Raman lines.
Electronic spectroscopy: Electronic transitions and selection rules, Frank Condon principle and electronic spectra of polyatomic molecules, Fluorescence and phosphorescence, solvent effects, absorption and intensity shifts,Calculationofabsorption maxima by Woodward-Fieser Rules.

Text Books:

1. Physical Chemistry by P.W. Atkins
2. Quantum Chemistry, by Ira N. Levine, Pentice Hall
3. Fundamentals of Molecular Spectroscopy by C.N. Banwell and E.M. McCash, Tata McGraw Hill.

Recommended Books:

1. Physical Chemistry by I. N. Levine
2. Thermodynamics for Chemist by S. Glasstone
3. Introduction to Quantum Chemistry by A.K. Chandra, Tata McGraw Hill.
4. Molecular Quantum Mechanics by P.W. Atkins & R.S. Friedman, Oxford University Press.
5. QuantumChemistry, byD.A. McQuarrie, VivaBooksPvt.Ltd.:NewDelhi
6. Introduction to Molecular Spectroscopy by G.M. Barrow, McGraw Hill.

Discipline Specific Elective
Course: DSE 104 A (Laboratory Course-I)
Credit 6
Marks - 150 (End Semester 90 + Internal Assessment 60)

L	T	P	C
0	0	6	6

Inorganic Lab I **Marks 25**

Preparation and characterization (viz. conductivity measurement, IR, UV-Vis) of the following complexes:
1. Potassium chromioxalate, $K_3[Cr(C_2O_4)_3]$
2. Reinecke's salt
3. Tris-(thiourea) copper(I) sulphate, $[Cu(tu)_3]_2SO_4.2H_2O$
4. Potassium chromithiocyanate
5. Chloropentamine Cobalt (III) chloride $[Co(NH_3)_5Cl]Cl_2$
6. NitropentamineCobalt(III) chloride $[Co(NO_2)(NH_3)_5]Cl_2$

Viva **Marks 5**

Organic Lab I **Marks 25**

1. Organic Estimation -
   i) Estimation of glucose and sucrose in a mixture.
   ii) Estimation of acetone by iodoform method.
   iii) Estimation of hydroxyl and amino groups by acetylation method.

2. Separation and identification of three components of organic compounds present in a mixture by TLC.

Viva **Marks 5**

Physical Lab I **Marks 25**

1. To determine the rate constant of hydrolysis of methyl acetate catalyzed by an acid and also the energy of activation.
2. To determine the velocity constant of hydrolysis of ethyl acetate by NaOH.
3. Determine the rate constant of inversion of cane sugar by analytical method.
4. Study the kinetics of the reaction between iodine and acetone in acidic medium by half-life period method and determine the order with respect to iodine and acetone.
5. Determine the molar mass of a polymer by viscometric method.

Viva **Marks 5**

Discipline Specific Elective
Course: DSE 104 B (Laboratory Course-I)
Credit 6
Marks - 150 (End Semester 90 + Internal Assessment 60)

L	T	P	C
0	0	6	6

Inorganic Lab I **Marks 25**

Preparation and characterization (viz. conductivity measurement, IR, UV-Vis) of the following complexes:

1. Sodium ferrioxalate, $Na_3[Fe(C_2O_4)_3]$ $9H_2O$
2. TetraamineCu(II)sulphate, $[Cu(NH_3)_4]SO_4.H_2O$
3. Hexa-amine Ni(II) chloride $[Ni(NH_3)_6]Cl_2$
2. Sodium Cobaltinitrite$Na_3[Co(NO_2)_6]$
5. NitritoPentamineCobalt(III) chloride, $[Co(ONO)(NH_3)_5]Cl_2$
6. Hexamine Co(III) sulphatepentahydrate, $[Co(NH_3)_6]_2(SO_4)_3.5H_2O$

Viva **Marks 5**

Organic Lab I **Marks 25**

1. Preparation of Green solvent : Ionic liquid and its use.

Viva **Marks 5**

Physical Lab I **Marks 25**

1. To determine the rate constant of hydrolysis of ethyl acetate catalyzed by an acid and also the energy of activation.
2. Study the complex formation between Cu^{2+} ion and ammonia by distribution method and find the composition of the complex.
3. To determine the radius of a molecule (glycerol) by viscosity measurements.
4. To study the kinetics of reaction between $K_2S_2O_8$ and KI.
   a) Determine the rate constant and order of the reaction
   b) Study the influence of ionic strength on the rate constant.
5. Determine the partial molar volume of ethanol by determining the densities of dilute aqueous solutions.

Viva **Marks 5**

Ability enhancement course (AEC)
Course: AEC 105 (Analytical Chemistry I)
Credit 2
Total Marks 50 (End Semester 30 + Internal Assessment 20)

L	T	P	C
2	0	0	2

Objectives:

1. To impart knowledge on the instrumentation of UV-Visible spectrometry and FT-IR.
2. To understand the basic principles of Thermal methods, Polarography, powder and single crystal XRD techniques.
3. To understand the applications of these instrumental techniques in studying various physical and chemical phenomena.

Expected learner outcome:

1. The students will gain the knowledge of basic instrumental parts of UV-Visible spectrometer and FT-IR.
2. The students will understand the working principles of Thermal methods, Polarography, X-Ray Diffractions.
3. The students will gain the knowledge of applications of mention techniques.
4. The students will able to characterize chemical compounds using UV-Visible spectrometry, FT-IR and powder and single crystal XRD techniques
5. The students will able analyze problem of physical and chemical phenomena using Thermal methods and Polarography techniques.

Unit I **Lecture 12, Marks 15**
Instrumentation and application of UV-Visible, IR, BET.Principles and applications of powder and single crystal XRD.

Unit II **Lecture 12, Marks 15**
Polarography: Basic principles, instrumentation and applications of cyclic voltammetry.
Thermal methods: Principles and applications of Thermogravimetry (TG), Derivativethermogravimetry (DTG), Differential thermal analysis (DTA) and Differential scanning calorimetry (DSC).

Text Books:

1. Instrumental Methods of Chemical Analysis - H Kaur, Pragati Prakashan

Recommended Books:

1. Solid State Chemistry and its Applications- A. R. West, Wiley India
2. Introduction to Thermal Analysis: Techniques and Applications- M.E. Brown, Springer

SEMESTER II

Course: Core 201(Inorganic chemistry-II)

Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To get a brief overview about inorganic reaction mechanism
2. To understand the application of group theory in Chemical Science.

Expected Learner Outcome:

1. Student will gather a thorough concept about the kinetics of inorganic reactions.
2. Student will understand the importance of group theory and applications in chemical science.

Unit I: Inorganic reaction mechanism **Lecture 16, Marks 20**

Lability and inertness, stability constant- formation constant of complexes, chelate effect, Thermodynamic and Kinetic stability; inert and labile complexes; Factor affecting stability, Correlation of stability constant with thermodynamic factors –G, H and S. Determination of stability constant –Jobs and Bjerrum's methods. Mechanism of ligand replacement reactions: Substitution reactions in octahedral [Cr(III), Co(III)] and square planar [Rh(I), Pt(II) and Pd(II)] complexes, Rate of water replacement reaction; Solvolysis and hydrolysis reaction; acid hydrolysis andbase hydrolysis reaction;Factors affecting the rate of substitution reaction, trans effect and its importance,theories of trans effect, idea concerning electron transfer reactions, inner and outer sphere reactions.

Unit II: Symmetry operation, elements of symmetry **Lecture 18, Marks 20**

Matrices and matrix representation of symmetry operations, Definition of Group, finite and infinite group.Examples of groups usinggeometrical object and symmetry operations.Symmetry elements as elements of group.Pointgroups.

Orthogonality theorem: reducible and irreducible representation, use of vectors andmathematical functions in group representation, Character table for molecular point group,construction of C_{2v} and C_{3v} Character table. Direct product representation. Projection operator,symmetry adapted linear combination (SALC) for C_{2v}, C_{3v}, D_{4h} and Td point group molecules.

Unit III: Chemical Application of Group Theory **Lecture 16, Marks 20**

Use of group theory in construction of hybrid Orbitals(d^2sp and sp^3 hybrids). Infrared absorption and Raman scattering spectroscopy, vibrationalmodes as bases for group representation, Symmetry selection rules for IR and Raman Spectra.Classification of vibrational modes and vibrational analysis. Orbital Symmetry and Chemicalreactions – Woodward and Hoffman rules for electrocyclic and cycloaddition reactions.

Text Books:

1. Inorganic Chemistry: Principles of structure and reactivity, 4^{th}Edition; J.E. Huheey, E.A. Keiter, R.L. Keiter, O.K. Medhi.

Recommended Books:

1. Advanced Inorganic Chemistry, 6^{th}Edition, F.A. Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann.
2. Inorganic Chemistry, K.F. Purcell and J.C. Kotz.

Course: Core 202 (Organic chemistry-II)
Credit 4
Total Marks 100 (End Semester 60 + Internal Assessment 40)

L T P C
3 1 0 4

Objectives:

1. To provide knowledge on
   a. isolation, characterization and synthesis of various natural compounds of biological importance
   b. heterocyclic compounds of biological and pharmaceutical importance
   c. applications of Mass spectrometry in combination with other spectroscopic techniques for analysis of molecular compounds.

Expected Learner Outcome:

1. Students will achieve insight on isolation, characterization and synthesis of various natural compounds of biological importance.
2. Students will acquire knowledge on different heterocylic compounds.
3. They will also be familiarized with mass spectrometric technique.

Unit I **Lecture 12, Marks 15**

Alkaloids :Occurance, classification, general methods of isolation, test for detection. Structure elucidation by physical and chemical methods and synthesis (including retrosynthetic approach) of :Piperine, Papaverine, Atropine and Morphine.
Terpenoids :Occurance and classification, isoprene rule, general methods of isolation. Biogenetic pathway of mono- and sesquiterpenes. Structure determination by physical and chemical methods and synthesis of the following:Acyclic monoterpenoid – Linalool.
Monocyclic monoterpenoid -Terpeneol, Menthol,
Bicyclic monoterpenoid: pinene, Camphor, Borneol.

Unit II **Lecture 12, Marks 15**

Carbohydrates : Structure, reaction and conformation of disaccharides – sucrose, maltose and lactose. Polysaccharides – starch and cellulose.Peptides and Proteins : Structure determination and synthesis of small peptides (di-, tri- and tetra-). Solid phase synthesis of peptides.Classification of proteins.Primary, secondary and tertiary structure of proteins.

Unit III **Lecture 13, Marks 15**

Heterocyclic Chemistry: Principles of heterocyclic synthesis involving cyclization and cyclo-addition reaction.Synthesis and properties of three, four and five membered heterocycles containing one and two heteroatoms viz., N, O and S (aziridine, oxirane, thiirane, azetidine, oxetane, thietane, pyrazole, isoxazole, isothiazole, imidazole, oxazole and thiazole). heterocycles. Elementary idea of Click Chemistry.

Unit IV **Lecture 13, Marks 15**

Mass spectrometry: Ion fragmentation mechanism, Base peak and molecular ion peak, metastable peak, instrumentation and techniques, ionization methods, isotopic distribution,

Application in determining the structure of organic and inorganic compounds
Spectroscopic methods in analysis of molecular composition/Structure: Use of IR, electronic, ^{1}H, ^{13}C & ^{31}P NMR, Mass spectrometry.

Text Books:

1. Organic Chemistry of Natural Products, Vol I and II, Gurdeep Chatwal, Himalaya Publishing House, Bombay.
2. Heterocyclic Chemistry : Synthesis, Reactions and Mechanisms – Raj K. Bansal, Wiley Eastern.

Recommended Books:

1. Chemistry of Organic Natural Products, Vol I and II , O.P. Agarwal, Goel Publishing House, Meerut.
2. The Alkaloids: K. W. Bentley.
3. Organic Chemistry, Vol- II, I.L. Finar
4. Heterocyclic Chemistry – T.L. Gilchrist, Longman Scientific and Technical/Pitman Publ. Ltd.
5. Spectrometric Identification of Organic Compounds – by Robert M. Silverstein, Francis X. Webster, David Kiemle, John Wiley & Sons.
6. Organic Spectroscopy – by William Kemp, Palgrave Macmillan.

Course: Core 203 (Physical chemistry-II)
Credit 4
Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To impart knowledge on the Schrodinger equation of Hydrogen atom and approximations applicable to more complex systems.
2. To understand the thermodynamics of adsorption, kinetics of heterogeneous catalysis, electrical aspects of surface chemistry, basics of reverse micelle and microemulsions.
3. To understand the concept of ensemble and to relate the macroscopic thermodynamic properties of a system to its microscopic properties through the application of statistical thermodynamics.

Expected Learner Outcome:

1. Students will be able to solve the Schrodinger equation for Hydrogen atom.
2. Student will be able to apply appropriate approximations to systems with more than one electron.
3. Students will understand the concepts of surface chemistry and will be able to solve problems regarding adsorption, heterogeneous catalysis, electro kinetic aspects of surface chemistry etc.
4. Students will be able to correlate the origin of the macroscopic thermodynamic properties in the microscopic properties of the constituent particles.
5. Students will be able to solve problems and calculate thermodynamic properties of simple systems using concepts of statistical thermodynamics.

Unit I: Quantum Chemistry-II **Lecture 24, Marks 30**

Hydrogen atom- Schrodinger equation, separation of relative coordinates, radial solution, probability and radial distribution function, angular solution, representation of orbitals, degeneracy, orbital and spin angular momentum.

Approximate methods: Variation theorem, Linear variation functions. Time independent Perturbation theory for non-degenerate systems (up to second order in energy); application to the helium atom.Hellmann-Feynmann theorem.

Antisymmetry Principle, Slater determinant, Term symbol, spectroscopic states.

Born-Oppenheimer approximation, LCAO-MO and VB treatment of the Hydrogen molecule and Hydrogen molecule ion, Comparison of Molecular Orbital and Valence Bond Methods.

Huckelmolecular orbital theory: Postulates, application to ethylene, butadiene, and benzene. Introduction to extended Huckel theory.

Unit II: Surface Chemistry **Lecture 12, Marks 15**

Thermodynamics of adsorption processes, Adsorption isotherms: Langmuir and BET. Determination of surface area of an adsorbent.

Capillary condensation – adsorption in micropores, hysteresis loop.

Kinetics and Mechanism of heterogeneous catalysis–Langmuir-Hinshelwood model, Eley-Riedel model, unimolecular and bimolecular surface reaction,
Chemisorption: Chemisorption on metals, semi-conducting oxides and insulator oxides.
Electrical aspects of surface chemistry, Electro kinetic phenomena, the structure of electrical double layer, Zeta potential and colloidal stability, Measurement of zeta potential.
Surfactants – definition and classification, micelle formation and determination of critical micelle concentration.
Reverse micelle and its application, solubilization, microemulsion.

Unit III: Statistical Thermodynamics **Lecture 14, Marks 15**

Probability and most probable distribution, distinguishable and indistinguishable particles, Concept of ensembles, partition functions and distributions, microcanonical, canonical and grand canonical ensembles, Boltzmann distribution, Elementary idea of Fermi-Dirac and Bose-Einstein distributions.
Ideal gases: Canonical partition function in terms of molecular partition function of non-interacting particles, Translational, rotational and vibrational partition functions. Absolute values of thermodynamic quantities (U,H,S,A) for ideal monoatomic and diatomic gases, heat capacity (C_v, C_p) of an ideal gas of linear and nonlinear molecules, chemical equilibrium.
Mono atomic Crystals - Einstein and Debye models.T^3 dependence of heat capacity of solids at low temperatures.
Numerical calculations of thermodynamic quantities for monoatomic, diatomic and polyatomic molecules.

Text Books:

1. Quantum Chemistry – Ira N. Levine, Pentice Hall
2. Statistical Mechanics – D.A. McQuarrie, Viva Books.
3. Physical Chemistry – P.W. Atkins, Oxford University Press.

Recommended Books:

1. Introduction to Quantum Chemistry – A.K. Chandra, Tata McGraw Hill.
2. Molecular Quantum Mechanics – P.W. Atkins & R.S. Friedman, Oxford University Press.
3. QuantumChemistry –D.A. McQuarrie, VivaBooksPvt.Ltd.:NewDelhi
4. Chemical Kinetics – K. J. Laidler, Pearson Education India.
5. Physical Chemistry of Surfaces – A. W. Adamson, Wiley India Pvt. Ltd.
6. An Introduction to Statistical Thermodynamics – T.L. Hill, Dover Books.
7. Statistical Thermodynamics – M.C. Gupta, Wiley Eastern Ltd.
8. Statistical Mechanics and its Chemical Applications – M. H. Everdell Academic Press.
9. Statistical Thermodynamics – B.J. McClelland, Chapman and Hall Ltd.
10. Fundamental of Statistical Thermodynamic – R.E. Sontagg& Gordon J.V.

Discipline Specific Elective
Course: DSE 204 A (Laboratory Course-II)
Credit 6
Marks - 150 (End Semester 90 + Internal Assessment 60)

L	T	P	C
0	0	6	6

Inorganic Lab 2 **Marks 25**

1. Estimation of Mg^{2+} and Ca^{2+} by complexometric method in different ores and from given solution with one / two components.
2. Estimation of alloys – Brass, Cu-Ni, etc.
3. Synthesis and characterization of nanoparticles by sol-gel and co-precipitation methods.

Viva **Marks 5**

Organic Lab 2 **Marks 25**

1. Separation and identification of amino acids present in a mixture by paper chromatography.

2. Organic Preparation -

One –step preparation

i) Cannizaro reaction of benzaldehyde (separation of benzyl alcohol and benzoic acid by solvent extraction)
ii) Oxidation of p-nitrotoluene to p-nitrobenzoic acid
iii) Reduction of benzophenone to benzhydrol
iv) Phthalic anhydride to phthalimide

Viva **Marks 5**

Physical Lab 2 **Marks 25**

1. To study hydrolysis of methyl acetate in presence of HCl and H_2SO_4 and hence determine the relative strength of the acids(use Guggenheim method)
   i) analytically.
   ii) polarimetrically.
2. Determine the equivalent conductivity of acetic acid at infinite dilution by Kohlrausch's method.
3. Determine the relative strength of acetic acid and monochloro acetic acid by conductance measurement.
4. Determine the specific rotation of sucrose and hence determine the unknown concentration of supplied solution by polarimetric measurements.
5. Determination of pH of a mixture of CH_3COOH and CH_3COONa, and hence determine the dissociation constant of the acid.
6. Preparation of conducting polymers and study of their electrical conductivity.

Viva **Marks 5**

Discipline Specific Elective
Course: DSE 204 B (Laboratory Course-II)
Credit 6
Marks 150 (End Semester 90 + Internal Assessment 60)

L	T	P	C
0	0	6	6

Inorganic Lab 2 **Marks 25**

1. Estimation of Zn^{2+} and Cu^{2+} by complexometric method in different ores and from given solution with one / two components.
2. Estimation of alloys – Bronze, Cu-Ni, etc.
3. Synthesis and characterization of nanoparticles by biogenic methods.

Viva **Marks 5**

Organic Lab 2 **Marks 25**

1. **Two –step preparation**
   i. p-nitrobenzene azo 2-naphthol (Para Red) from p-nitroaniline
   ii. Benzanilide from benzophenone
   iii. Dibenzyl from benzoin

2. Preparation of Green reagent: TetrabutylammoniumTribromide (TBATB) and its use

Viva **Marks 5**

Physical Lab 2 **Marks 25**

1. Determine the specific rotation of sucrose and hence determine the unknown concentration of supplied solution by polarimetric measurements.
2. Determine the amount of each component of the following ternary mixture by conductometric titration.
   i) HCl, CH_3COOH, $CuSO_4$
   ii) HCl, NaCl, NH_4Cl
3. Determine the ionization constant of acetic acid by conductivity method.
4. Determination of Critical Micelle Concentration (CMC) of Sodium dodecyl sulphate (SDS) by surface tension measurement.
5. To find the stability constant of the co-ordination compound formed between Cu^{2+} and 5-sulphosalicylic acid.
6. Establish the order reaction for $K_2C_2O_4 + 2HgCl_2 \rightarrow Hg_2Cl_2 + 2KCl + 2CO_2$ by the method of ratio variation.

Viva **Marks 5**

General Elective-I
Course: GE 205 (Materials Chemistry)
Credit 4
Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To provide the students a brief exposure about materials of technological importance
2. To provide knowledge about synthesis and structural properties of nanomaterials.

Expected Learner Outcome:

1. Students will gather a brief knowledge about synthesis, characterization techniques and applications of various types of materials.
2. Student will learn state of the art knowledge about new materials.

Unit I: Materials of technological importance **Lecture 15, Marks 20**

Introduction to Bio-inspired/Bio-mimetic materials. Bio-materials: types, properties, design, preparation and application. Structural, functional bio-mimetics, nano-biomimetics, Introduction to bio-sensors, nano-biosensors; technological importance.Principles, examples and current status.

Unit II: Polymer materials **Lecture 18, Marks 20**

Classification of polymers, Molecular forces and chemical bonding in polymers, Texture of Polymers. Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point. Physical, thermal, Flow & Mechanical Properties of polymers.Conducting polymers- Introduction, conduction mechanism, polyaniline (PANI), polyacetylene, polyparaphenylene and polypyrrole, applications of conducting polymers, Ion-exchange resins and their applications.polymer-matrix composites. Ceramic & Refractory: Introduction, classification, properties, raw materials, manufacturing and applications.

Unit III: Nanostructured materials **Lecture 17, Marks 20**

Introduction to Nanoscience and Nanotechnology, influence of nano over micro/macro. 1D, 2D and 3D nanostructured materials, Quantum Dots shell structures, mechanical-physical-chemical properties, Quantum confinement effect and Surface plasmon resonance. Synthesis and modification of nanoparticles**:** Top-Down and Bottom-Up approach, experimental procedure (coprecipitation, Sol-gel, Hydrothermal, colloidal etc.), Properties of precipitates and precipitating reagents: Colloidal and Crystalline Precipitates, nucleation (homogeneous and heterogeneous), crystal growth, morphology dependence properties. Introduction to surface active agents, types of surfactants. Basic characterizations for structural purity and morphology study. Applications of metal oxide and semiconductor nanoparticles in catalysis (photocatalysis, electrocatalysis etc.) and energy.

Text Books:

1. Solid State Chemistry and its applications A.R. West, John Wiley & Sons
2. Polymer Science by V.R. Gowarikar, N. V. Viswanathan and Jayadev Sreedhar

Recommended Books:

1. Inorganic Chemistry, Shriver & Atkins, 5^{th} Edition Oxford
2. Introduction to Polymer by R. J. Young and P. A. Lovell

SEMESTER III

Course: Core 301 (Inorganic chemistry-III)

Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To give a brief knowledge about properties of d and f block elements
2. To provide basic concept about spectroscopic methods in Inorganic Chemistry

Expected Learner Outcome:

1. To enable our students to solve spectroscopic problems for Inorganic molecules.
2. Student will gather thorough knowledge about the chemistry of d and f block elements.

Unit I: Chemistry of Lanthanides and Actinides **Lecture 8, Marks 08**

Electronic configuration, lanthanidecontraction, separation of lanthanides, Magnetic and spectral properties of lanthanides and actinides,lanthanide shift reagents.Stability of lanthanide and actinide complexes.

Unit II: Properties of transition metal complexes **Lecture 12, Marks 16**

(A) Transition metals and periodic properties. Transition metal donor-acceptor compounds,Coordination number and geometries, 18-electron rule, Stability of metal complexes, commonligands and complexes, Stereochemically non-rigid systems.

Introduction to transition metal organometallic chemistry: Metal carbon bond formation,18 and 16 electron organometallic complexes. Isolobel analogy in organometallic compounds. Bonding in organotransitionmetal compounds: Metal carbonyls, metal olefins, metal carbene, Role of co-ligands likephosphine, arsine, stibine, N_2, O_2 and NO. Oxidative addition, reductive elimination andβ-elimination reaction.

(B) Electronic spectra and magnetic properties of transition metals complexes:Electronic states and terms for transition metals. Selection rules,Orgel diagram and TanabeSugano diagrams: Application in transition metal electronic spectroscopy. Electronic spectraand structure, d-d and charge transfer transitions.

Unit III **Lecture 22**

(A) **Application of NMR spectroscopy** (^{1}H, ^{31}P and ^{19}F) : Chemical shift, factorscontributing to chemical shift, spin-spin coupling and its implication to structuredetermination; simplification of complex spectra; Use of ^{31}P and ^{19}F NMR incoordination chemistry: metal-ligand interaction; isomer determination; evaluation ofstereo chemical non-rigidity in molecules; NMR spectra of paramagnetic compounds.

Marks 7

(B) **ESR spectroscopy**: Principle, resonance condition, Origin of g-value, spin orbit coupling, Kramer degeneracy, zero-field splitting, hyperfine &superhyper interaction, line width and application of ESR in organic radicals and transition metal coordination complexes (e.g., d^1, d^3 and d^9).

Marks 7

(C) **Mossbauer spectroscopy**: Principle of Mossbauer spectroscopy, Instrumentation,Application of Mossbauer spectroscopy: the isomer shift, magnetic interaction, quadruplesplitting, line with. Application to iron to iron and tin compounds.

Marks 6

(D) **NQR spectroscopy**: Principle of NQR, Quadruple constant, Application of NQRspectroscopy.

Marks 5

(E) Introduction to Photoelectron Spectroscopy : Auger electron spectroscopy.

Marks 4

Unit IV: Magnetochemistry **Lecture 8, Marks 7**

Types of magnetic bodies (eg, Diamagnetic, Paramagnetic, ferromagnetic and antiferromagnetic), antiferromagnetic coupling, Magnetic properties based on crystal field theory:spin only magnetic moments, spin-state equilibrium in octahedral stereochemistry:cross-over region, quenching of orbital magnetic moment by CF, orbital contribution,effect of temperature on magnetic behaviour, magnetic properties of octahedral,tetrahedral, tetragonally distorted octahedral and sequence planer complexes.

Text Books:

1. Inorganic Chemistry, Shriver & Atkins, 5^{th} Edition Oxford
2. Fundamentals of Molecular Spectroscopy: C.N. Banwell and E.M. McCash, Tata McGraw Hills

Recommended Books:

1. Inorganic Chemistry, W.W. Porterfield, 2nd Edition, Academic Press
2. Physical Methods for Chemist, Russell S. Drago
3. Elements of Magnetochemistry, R. L. Dutta and A Syamal

Course: Core 302 (Organic chemistry-III)
Credit 4
Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To impart basic knowledge on petroleum technology.
2. To gain knowledge on conformational behavior of organic molecules.
3. To acquire knowledge on various redox reagents.

Expected Learner Outcome:

1. Students will understand the basics of petroleum industry.
2. They will get a stereochemical insight of different organic molecules.
3. They will be familiarized with different oxidative and reductive reaction components.

Unit I: Petroleum Technology **Lecture 12, Marks 15**

'Upstream'— the exploration and production sector of the industry; survey, exploration, drilling, drilling fluid, well stimulation, enhanced oil recovery, transportation and storage.
'Downstream'—the sector which deals with refining and processing of crude oil and gas products; petroleum product profile, crude oil evaluation, natural gas and petroleum products, processing and purifying/refining of crude oil and natural gas, reforming.
Environmental management and corrosion prevention in petroleum technology.

Unit II: Stereochemistry **Lecture 12, Marks 15**

Conformational analysis of disubstitutedcyclohexanes, cyclohexene, cyclohexanone, 2-alkyl, 3-alkyl, and 4-alkyl ketone effects. $A^{1,2}$ and $A^{1,3}$ strains. Conformation of fused systems - decalins and perhydrophenanthrenes.Effects of conformation on reactivity and mechanism of basic organic reactions of 6-membered ring compounds.Chiroptical properties - Optical rotatory dispersion, circular birefringence, circular dichroism, axial haloketone rule, octane rule.

Unit III: Oxidation **Lecture 13, Marks 15**

(i) of carbon-carbon double bond : dihydroxylation by $KMnO_4$, OsO_4(including Sharpless asymmetric dihydroxylation), iodine and silver carboxylate (Woodward and Prevost condition) and peroxy acid. Allylic and benzylic oxidation of alkene: Use of $SeO_2$and DDQ.
(ii) of alcohols : Use of Cr(VI) based reagents (PCC, PDC), DMSO-based reagents (Swern, Pfitzner-Moffatt and Albright – Goldman), Tetrapropyl ammonium perruthenate (TPAP);
(iii) of 1,2- diols.

Unit IV: Reduction **Lecture 13, Marks 15**

(i) by catalytic hydrogenation : both heterogeneous (H_2/Pd-C, H_2/Pt_2O, Lindlar's and Rosendmund's reduction) and homogeneous (Wilkinson catalyst),
(ii) by modified hydride transfer reagents (Lithium trialkoxyaluminium hydrides, DIBAL, $NaCNBH_4$, SMEAH (Red Al), Superhydride and Selectrides, 9-BBN
(iii) by dissolving metal (alkali metals in liquid ammonia) and (iv) by diimide.

Electrooxidation and reduction, Use of Baker's Yeast.

Text Books:

1. Stereochemistry of Organic Compounds – D. Nasipuri, Wiley Eastern
2. Modern Methods of Organic Synthesis – Carruthers and Coldham, Cambridge University Press
3. Fundamentals of Oil & Gas Industry for Beginners – Samir Dalvi, Notion Press

Recommended Books:

1. Stereochemistry of Carbon Compounds – Earnest E. Eliel, Tata McGraw Hill
2. Stereochemistry of Carbon Compounds – SubrataSengupta, New Central Book agency, Kolkata
3. Stereochemistry and Mechanism through Solved Problems- P.S. Kalsi, New Age International Publishers
4. Organic Synthesis – M.B. Smith, McGraw Hill. (Reference book)
5. Principles of Organic Synthesis – R.O.C. Norman and J M Coxon
6. Advanced Organic Chemistry Part A and B : Carey and Sundberg
7. Organic Synthesis – J. Singh and L.D.S.Yadav, PragatiPrakashan
8. Application of Redox and Reagents in Organic Synthesis- R.K. Kar, New Central Book Agency
9. Fundamentals of Organic Synthesis : The Retrosynthetic Analysis - R.K. Kar, NCBA
10. Synthetic Approaches in Organic Chemistry – R.K. Bansal- Narosa Publishing House, New Delhi
11. Modern Synthetic Reactions – H.O. House, W.A. Benjamin, NY
12. Oil and Gas Production Handbook: an Introduction to Oil and Gas Production, Transport, Refining and Petrochemical Devold Havard

Course: Core 303 (Physical chemistry-III)
Credit 4
Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To impart knowledge on theories of reaction kinetics and dynamics, Unimolecular reaction kinetics, reactions in solutions, fast reactions and enzyme catalysis.
2. To understand the applications of Nernst equation, concepts of ion-ion and ion-solvent interactions.
3. To understand the structure and symmetry of crystalline solids, its defects and applications of band theory.

Expected Learner Outcome:

1. Students will be able to understand the theories of reaction kinetics and will be able to solve problems related to different types of reaction kinetics and catalysis.
2. Students will gain the skills to solve the problems regarding galvanic cells, electrolytic cells.
3. Students will understand the concepts of ion pairs and ion associations in electrolytic solutions, applications of Debye Huckel Theory and Bjerrum hypothesis.
4. Students will gain knowledge about structures of crystalline solids, importance of crystal defects, and will understand the applications of band theory to electrical and magnetic properties of solids.

Unit I: Chemical Kinetics and Reaction Dynamics **Lecture 22, Marks 30**

Methods of determining rate laws, Activated complex theory, structure of transition state, Eyring equation, chain reactions and oscillatory reaction, steady state approximation.

Unimolecular reactions – Drawbacks of Lindemann theory, Hinshelwood, Kassel, Rice and Ramsperger theory, Stater's Theory.

Relaxation kinetics – linearized rate equation, relaxation time (in single step reaction) ; determination of relaxation time and rate constant, Methods of studying fast reaction – flow method, temperature jump and pressure jump method, NMR method, flash photolysis.

Reactions in solution – Factors determining reaction rates in solution, reactions involving ion-ion and ion-dipoles reaction; influence of solvent, ionic strength and pressure on the reactions in solution.

Rate of enzyme catalyst reaction, Michaelis-Menten equation; temperature, pH and concentration dependence of enzyme catalysed reactions; acid-base catalysis and acidity function.

Kinetics of polymerization.

Unit II: **Electrochemistry** **Lecture 14, Marks 15**

General electrochemical concepts. Introduction to electrochemistry: thermodynamics, electrode potentials, galvanic and electrolytic cells, electrode kinetics, dynamic electrochemistry, mass transport by migration, diffusion and convection, diffusion layers.

Ion-Solvent Interaction: Ion-Dipole, Ion-quadruple, Ion-Induced Dipole Interaction, Ion-Association: Bjerrums hypothesis, Thermodynamics of ion-pairing, relation between Debye-Huckel free ion and Bjerrums ion-pair.
Polarizable and non polarizable electrodes. Inner and Outer potential, Thermodynamics of Electrified Interfaces: Surface Excess and its determination.
Electrical double layer (DL): HP/ GC/ Stern model. Potential variation in DL and capacity of DL.

Unit III: Solid State Chemistry **Lecture 14, Marks 15**

Crystal Systems, Brief description of crystal symmetry and point group (Hermann Mauguin symbols), Space group (Monoclinic and Triclinic systems). Crystal defects (Frenkel and Schottky), line (edge and screw dislocations) and plane defects (grain boundaries and staking fault), Octahedral and tetrahedral voids. Electronic structure: Band theory of solids, electrical and magnetic properties of solids.

Text Books:

1. Chemical Kinetics – K. J. Laidler, Pearson Education India.
2. Modern Electrochemistry – Vol I, II by J. O. M. Bockris& A. K. N. Reddy
3. Solid State Chemistry and its Application – A. R. West, Wiley India.

Recommended Books:

1. Chemical Kinetics and Reaction Dynamics – P. L. Houston, Dover Publications
2. Kinetics and Mechanism – A. A. Pearson, R. G. Frost, John Wiley and Sons
3. Electrochemical Methods: Fundamentals and Applications, A. J. Bard, L. R. Faulkner, John Wiley and Sons.
4. An Introduction to Electrochemistry – S. Glasstone, East West Press.
5. Physical Chemistry – P.W. Atkins, Oxford University Press.
6. Solid State Chemistry – D. K. Chakravorty
7. Principles of Solid State – H. V. Keer, New Age International.

Course: DSE 304 A (Laboratory Course)
Credit 6
Marks 150 (End Semester 90 + Internal Assessment 60)

L T P C
0 0 6 6

Inorganic Lab III **Marks 25**

1. Synthesis and characterization (melting point, conductivity, IR, UV-vis etc.) of trans-triglycinatoCu(II) monohydrate and estimate the percentage of 'Cu' in the synthesized compound.
2. Synthesis and characterization of Schiff-base ligands and their metal complexes.
3. Synthesis and characterization of magnetic nanoparticles by surfactant assisted methods.

Viva **Marks 5**

Organic Lab III **Marks 25**

1. Preparation, purification (by TLC) and spectroscopic identification (UV and IR) of the prepared organic compounds and (B) Estimation]

Preparation:

i. Benzilic acid from benzoin via benzyl (Benzilic acid rearrangement)
iiBenzanilide from benzophenone via oxime (Beckman rearrangement)
iii. Indigo from anthranilic acid via phenylglycine-o-carboxylic acid and indoxyl
iv. Sandmeyer reaction-
(a) ortho-Chlorotoluene from ortho-toluidine (steam distillation of the product)
(b) Acridone from anthranilic acid via o-chlorobenzoic acid and N-phenylanthranilic acid
v. Sulphanilamide from acetanilide via p-acetamidobenzenesulphonylchloride and p-acetamidobenzenesulphonamide
vi. Pinacolone from benzophenone via pinacol (Pinacolpinacolone rearrangement)

Viva **Marks 5**

Physical Lab III **Marks 25**

1. Determination of hydrolysis constant of aniline hydrochloride by pH measurements.
2. Determine the strengths of the components of the following mixtures by conductometric titration
   a) Hydrochloric acid and acetic acid
   b) Sulphuric acid and copper sulphate
3. Determine the strengths of HCl and CH_3COOH in a given mixtures by pH-metric titration.
4. Verify Beer's law and determine the unknown concentration of supplied solutions like $KMnO_4$ / $K_2Cr_2O_7$
5. Determine the composition of iron-salicylic acid complex spectrophotometrically by Job's method.
6. Least squares fitting and plotting linear and exponential graphs performing theoretical calculations using a computer

Viva **Marks 5**

Course: DSE 304 B (Laboratory Course)
Credit 6
Marks 150 (End Semester 90 + Internal Assessment 60)

L	T	P	C
0	0	6	6

Inorganic Lab-III **Marks 25**

1. Synthesis and characterization (melting point, conductivity, IR, UV-vis etc.) of Ni-DMG complex and estimate the percentage of nickel in the synthesized compound.
2. Synthesis and characterization of Schiff-base ligands and their metal complexes.
3. Synthesis and characterization of metal and metal oxide nanoparticles by surfactant assisted methods.

Viva **Marks 5**

Organic Lab III **Marks 25**

1. ***Estimation:***
   i) Estimation of glycine by formalin method
   ii) Estimation of halogen by fusion method
   iii) Estimation of hydroxyl and amino groups by acetylation method

2. Synthesis of Deep Eutectic Solvents (DES) and its use.
3. Green synthesis of Coumarin derivative (clay catalyzed).
4. Benzoin condensation using Green catalysts (co-enzymes).

Viva **Marks 5**

Physical Lab III **Marks: 25**

1. Determine the composition of the binary mixture ($K_2Cr_2O_7$ and $KMnO_4$) by spectroscopic method (MLRA).
2. Determine the indicator constant of methyl red.
3. Investigate the reaction between H_2O_2 and HI (clock reaction). Determine the energy of activation
4. Determination of molecular surface energy and the association factor for ethanol.
5. Study and compare the spectroscopic properties of acetone in different solvents. Comment on the energy of hydrogen bonding.
6. Perform theoretical calculations using a computer
   a) Charge density distribution and shapes of s and p orbitals.
   b) Potential energy diagram of hydrogen molecule ion

Viva **Marks 5**

Course: GE 305(Green and Sustainable Chemistry)

Credit 4

Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To develop preliminary knowledge on the necessity of green chemistry practices.
2. To familiarize students with various greener approaches in chemical transformations.

Expected Learner Outcome:

1. Students will understand the importance of practicing green chemistry principles in synthetic laboratories.
2. Through this course they will be able to design greener methodologies for chemical transformations.

Unit I: Introduction to Green Chemistry **Lectures 3, Marks 5**

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry.Limitations? Obstacles in the pursuit of the goals of Green Chemistry; E-factor.

Unit II: Principles of Green Chemistry and Designing a Chemical synthesis

Lectures 15, Marks 25

Twelve principles of Green Chemistry with their explanations and examples and special emphasis on the following:

i. Designing a green synthesis using these principles;Prevention of waste/ byproducts.
ii. Atom Economy, calculation of atom economy for chemical transformations.
iii. Prevention/ minimization of hazardous/ toxic products.
iv. Green solvents- supercritical fluids, water, ionic liquids and PEGs as green solvents for organic reactions.
v. Energy requirements for reactions- alternative sources of energy: use of microwaves and ultrasonic energy.
vi. Selection of starting materials; carbohydrates, CO_2 and vegetable oils as green starting materials.
vii. Use of catalytic reagents in preference to stoichiometric reagents; solid acids catalysis- use of zeolite, hydrotalcite etc. PTC catalyzed green reactions; co-enzymes as catalysts.
viii. Prevention of chemical accidents designing greener processes, inherent safer design.

Unit III: Examples of Green Reagents/ Synthesis/ Reactions **Lectures 15, Marks 25**

1. Green synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate, paracetamol, ibuprofen.

2. Microwave assisted reactions: Microwave assisted reactions in water (oxidation of toluene to benzoic acid, oxidation of alcohols); microwave assisted reactions in organic solvents (Diels-Alder reaction and Decarboxylation); Microwave assisted solvent-free reactions (solid state reaction)- Michael addition and Knoevenagel reaction)

3. Ultrasound assisted reactions: Grignard reaction, Ulmann coupling and Cannizaro reaction under sonication.
4. Dimethyl carbonate (DMC) and Tetrabutylammoniumtribromide (TBATB) as green reagents in organic synthesis.

Unit IV: Green chemistry in sustainable development **Lectures 3, Marks 5**
Oxidation reagents and catalysts; multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions.

Text Books:

1. B. Saikia and D. Sarma, A textbook on Green Chemistry, Kalyani Publications (2017).

Reference Books:

1. P. T. Anastas & J. K. Warner: Oxford Green Theory and Practical, University Press (1998).
2. A. S. Matlack: Introduction to Green Chemistry, Marcel Dekker (2001).
3. M. C. Cann& M. E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
4. M. A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).

Course: AEC 306 (Analytical Chemistry II)
Credit 2
Total Marks 50 (End Semester 30 + Internal Assessment 20)

L	T	P	C
2	0	0	2

Objectives:

1. To impart fundamental knowledge of different Chromatographic methods and their applications.
2. To understand the working principle of Electron Microscopy and Atomic Force Microscopy.

Expected learner outcome:

1. Students will understand the principle of Chromatographic methods, Electron Microscopy and Atomic Force Microscopy
2. Students will learn to separate mixtures of chemical compounds using Chromatographic methods.
3. Student will able to investigate physical and chemical phenomena by Electron Microscopy and Atomic Force Microscopy.

Unit I: **Lecture 12, Marks 15**
Chromatographic methods: Adsorption, liquid-liquid partition, ion–exchange, HPLC, gelpermeation chromatography and gas chromatography, HPTLC, Flash chromatography.

Unit II: **Lecture 13, Marks 15**
Transmission Electron Microscopy (TEM),Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM)

Text Books:

1. Instrumental Methods of Chemical Analysis - H Kaur, Pragati Prakashan

Recommended Books:

1. Introduction to Thermal Analysis: Techniques and Applications- M.E. Brown, Springer
2. Introduction to Instrumental analysis – R.D. Braun, McGraw Hill.

SEMESTER IV

Course: Core 401 (Inorganic chemistry-IV)

Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To provide a thorough knowledge about Inorganic reaction mechanism
2. To impart knowledge about basic Organometallic Chemistry.
3. To introduce the student with various catalytic processes, both homogeneous and heterogeneous systems.

Expected Learner Outcome:

1. Student will gain advanced knowledge on various types of organometallic complexes and their utility as catalysts in various organic reactions.

Unit I: Inorganic Reactions **Lecture 24**

(A) Electron transfer reaction: Rearrangement of Precursor complex and electron transfer; Nature of bridging ligand;2-electron transfer; Synthesis of coordination compounds using redox reaction;complementary and non conplementary reaction; Oscillating reactions; Template effect andmacrocyclic ligands; reactions of coordinated ligands. Synthesis of coordination compound by substitution reactions;Isomerization and racemization of tris-chelate complexes; Molecular rearrangement infour-coordinated and six-coordinated complex. **Marks 20**

(B) Photochemical reactions of Transition metals: Basic photochemical processes, photosubstitution reactions, photoredox reactions, ligand photoreactions, photoreactions and solar energy conversion. **Marks 8**

Unit II:Organotransition metal Chemistry **Lecture 14, Marks 16**

Structure and bonding of *pi* bonded organometallic compounds including carbonyls, nitrosyls, tertiary phosphines, hydrides, alkene, alkyne, cyclobutadiene, cyclopentadiene, arene compounds. Metal-carbon multiple bonds.Fluxional organometallic compounds including π-allyl complexes.Carbon σ donors: Synthesis of metal alkyls and aryls, direct reaction of a metal with organic halides, reaction of anionic alkylating agents with metal halides, Metallation reactions.

Unit III: Homogeneous and Heterogeneous catalysis **Lecture 12, Marks 16**

Introduction and definition; alkene metathesis (olefins); alkene hydrogenation, carbonylation, hydroformylation, alkene oligomerization, polymerization, polymer supported and biphasic catalysis, transition metal organometallic clusters, surfaces and interactions with adsorbates, Fischer-Tropsch carbon chain growth; use of ZSM-5 for organic transformations; Suzuki-Miyaura, Heck and Sonogashira cross-coupling reactions. Activation of small molecules (O_2, H_2, N_2, CO and CO_2).

Text Books:

1. Inorganic Chemistry: Principles of structure and reactivity, 4th Edition; J.E. Huheey, E.A. Keiter, R.L. Keiter, O.K. Medhi

Recommended Books:

1. Advanced Inorganic Chemistry, 6th Edition, F.A. Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann.
2. Inorganic Chemistry, K.F. Purcell and J.C. Kotz.
3. Basic Organometallic Chemistry, concept, Synthesis and applications, B. D. Gupta and A. J. Elias; Universities Press, 2010
4. Organometallic Chemistry of Transition Metals, R. H. Crabtree; John Wiley & Sons, 2001

Course: Core 402 (Inorganic chemistry-V)
Credit 4
Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To provide general knowledge about nuclear chemistry
2. To provide exposure to the students about cluster chemistry.
3. To gain preliminary knowledge about Supramolecular Chemistry.
4. To provide advance knowledge on the area of nanomaterials.

Expected Learner Outcome:

1. Student will learn the depth of Inorganic Chemistry in a more holistic way so that they can compete for various type of competitive examinations.

Unit I: Nuclear Chemistry **Lecture 8, Marks 08**

Nuclear structure and nuclear stability, Radioactivity and Nuclear reactions, fission and fusion, radio-analytical techniques and activation analysis.

Unit II: Clusters **Lecture 10 Marks 12**

Definition of clusters, Low and high nuclearity metal carbonyl and metal halide clusters,bimetallic clusters. Closed shell electronic requirements for clustercompounds, introduction to tensor surface harmonic theory of clusters. Organization of neutral boron hydrides, anionic borane, carboranes and metallocarboranes.Synthesis and properties of C_{60}.

Unit III: Supramolecular Chemistry **Lecture 6 Marks 06**

Introduction to Supramolecular Chemistry, Concepts of host guest chemistry, classification,Non-covalent interactions, Molecular recognition,Supramolecular reactivity and catalysis, Effects of medium, Chiral recognition.

Unit IV: Materials Chemistry **Lecture 26**

(A) Synthesis and modification of inorganic solids**:** General principle of solid state reaction, experimental procedure (coprecipitation, Sol-gel,Hydrothermal, Intercalation etc.), Preparation of crystalline materials, nucleation, crystal growth,Graphite and zirconium intercalation compounds, transition metal chalcogenide, thin films, growth of single crystals. Catalyst immobilization onto silica andclay surfaces and applications, pillaring of certain clays.Electronic and optical properties ofsome inorganic and organic solids (Solid electrolytes, Inorganic coloured solids, white andblack pigments).Design and properties of composites, polymer matrix andcarbon-carbon composites.Brief idea about drilling muds.

Marks 18

(B) Introduction to physics and Chemistry of solid materials, energy bands: conductor, semiconductor and insulator; Graphite, graphene-oxide, diamond. Size and morphology dependence properties. Methods of measuring properties: crystallography, size of particles, surface structure.

Synthesis and Properties of nanomaterials: Metal oxide, semiconducting nanoparticles.Nanoclusters, Composites and Nanotubes. Top-Down and Bottom-Up approach, Quantum confinement effect and Surface plasmon resonance.
Application of various solid materials in fuel cell, photovoltaic cell, in electrochemistry as electrode materials (capacitor material), photocatalysis and chemical sensors.

Marks 16

Text Books:

1. Introduction to Cluster Chemistry, D. M. P. Mingos and D. J. Wales, Prantice- Hall, 1990

Recommended Books:

1. Supramolecular Chemistry, Jonathan W. Steed and Jerry L. Atwood
2. Solid State Chemistry and its applications, by A.R. West, Plenum.
3. Inorganic Chemistry, Shriver & Atkins, 5th Edition Oxford

Course: Core 403 (Organic chemistry-IV)

Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To impart knowledge on different classes of pericyclic reactions.
2. To develop knowledge on organic photochemical reactions- particularly of carbonyl compounds and alkenes.
3. To understand mechanisms and applications of certain name reactions of C-C, C-N etc. bond formation type.

Expected Learner Outcome:

1. Students will understand the stereochemical aspects of different classes of pericyclic reactions.
2. They will gain knowledge on photochemical behavior of carbonyl compounds and alkenens.
3. Students will learn the mechanistic aspects of various name reactions.

Unit I **Lecture 15, Marks 20**

Pericyclic reactions – Classification of pericyclic reactions, FMO method, Orbital symmetry correlation method, PMO method for the explanation of pericyclic reactions under thermal and photochemical conditions; Cycloaddition reactions: [2+2], [4+2], [6+4] cycloadditions, 1,3-dipolar cycloadditions; the ene reaction, cheletropic reactions, Sigmatropic rearrangement – [m+n] sigmatropic shifts of hydrogen and carbon, Cope and Claisen rearrangement. Electrocyclic reactions, Stereoselectivity and regioselectivity of pericyclic reactions.

Unit II **Lecture 15, Marks 20**

Photochemistry of organic compounds – Jablonski diagram, photosensitization, quenching. Olefinic photochemistry – Photostereomutation of cis-trans isomers, optical pumping, photochemistry of conjugated dienes – cycloaddition and dimerisation of butadiene, Photochemistry of vision.

Photochemistry of carbonyl compounds – Norrish type I and type II processes, photoreduction of saturated aryl, alkyl and unsaturated ketones, Paterno-Buchi reaction,

Photorearrangements – di--methane rearrangement and rearrangement of cyclohexadienes, Reaction of singlet oxygen, photooxidation.

Unit III **Lecture 10, Marks 10**

Study of the following reactions, their mechanism and synthetic utility Henry reaction, Mitsunobu reaction, Corey-Nicolaoumacrolactonization, BaylisHilman reaction, Vilsmeier–Haack reaction, Wohl Ziegler allylicbromination, Barton reaction.

Unit IV **Lecture 10, Marks 10**

Elementary idea of PASE synthesis, Combinatorial Chemistry, Parallel synthesis, Microwave synthesis.Nanocatalysis in Organic synthesis.Olefin metathesis.

Text Books:

1. Frontier Orbitals and Organic Chemical Reaction – Ian Flaming, John Wiley
2. Photochemistry and PericyclicReactions : J Singh and J Singh, New Age International Publishers

Recommended Books:

1. Advanced Organic Chemistry Part A and B - Carey and Sundberg
2. Organic Photochemistry – J.M. Coxton and B. Halton, Cambridge University Press.
3. Introductory Photochemistry – A. Cox and T.J. Kemp, McGraw Hill
4. Elements of organic photochemistry – Dwaine O. Cown and Ronald L. Driske, Plenum Press, New York and London
5. Fundamentals of Photochemistry – K.K. Rohatgi-Mukherji, Wiley Eastern

Course: Core 404 (Organic chemistry-V)
Credit 4
Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To impart knowledge on action of various drugs, QSAR concept and interaction mechanism.
2. To introduce different biomolecules and their bio-functioning mechanisms.

Expected Learner Oucome:

1. Students will understand the action of different drugs, factors affecting their bioactivity and mode of action.
2. Students will gain knowledge on biomolecules and their role in life processes.

Unit I: Drugs **Lecture 15, Marks 15**

Definition of drugs and factors affecting their bioactivity; Definition of chemotherapeutic index and therapeutic index. Quantitative structure activity relationship (QSAR).Concepts of drug receptor, theoretical aspects of drug receptor interaction.Drug introduction, Metabolism, Excretion.Introduction to designing of drugs; Structural modification of drugs.Introduction to combinatorial library of drugs.

Sulphadrugs: Historical significance of sulpha drugs as antibacterial agent, Sulphanilamide and other important sulpha drugs and their mode of action.

Antibiotics : Introduction and classification, Structure action relationship and mode of action of penicillin, semisynthetic penicillins, streptomycin, tetracyclins. Antimalarials: Introduction and classification, human malaria and plasmodia, mepaquine, trimethopriim and mefloquine – their structure and activity as antimalarials. Artemisinin and its derivatives, structure-action relationship.

Drugs used for treatment of cancer and tuberculosis and recent developments.

Unit II: Bio-Chemistry **Lecture 13, Marks 15**

Enzymes and Co-enzymes : Classification of enzymes; Chemical nature of enzyme, Specificity of enzyme, Mechanism of enzyme action, Factors effecting enzyme action, Mechanism of action of chymotrypsin.Co-enzymes, co-factors, prosthetic groups: Mechanism of action of NAD^+, $NADP^+$, FMN, FAD. Functions of ATP.

Nucleic acids: Review on chemical constitution and biological role of nucleic acids. Double heical structure of DNA.Chemical basis of heredity, Genetic code, Replication of DNA.Transcription and translation.Biosynthesis of proteins, Chemical synthesis of DNA, PCR.

Unit III: Organic synthesis I **Lecture 12, Marks 15**

Organometallic reagents in formation of carbon-carbon bonds: Organopalladium in C-C formation (Heck reaction, Stille, Suzuki, Sonogashira and Negishi Coupling).Formation of C=C bonds by elimination reactions, syn elimination; Wittig and related reactions, McMurry reaction, Peterson olefination, Julia reaction and Tebbeolefination. Use of organosulphur compounds for reversal of polarity (Corey-SeebachUmpolung).Allylic activation by - allyl Ni and - allylPd complexes.

Unit IV: Organic synthesis II **Lecture 10, Marks 15**

Application of Enamines, Hydroboration and trialkylsilyl halides in organic synthesis. Use of the following reagents: Organotin (TBTH), Lithium Diisopropyl Amide (LDA), Dicyclohexylcarbodiimide, Dicyanodichloroquinone (DDQ), Dimethyl dioxirane (DDO), lipase and other reagents of organozinc and organocopper.

Text Books:

1. The Organic Chemistry of Drug Design and Drug Action – Richard B.Silverman, Elsevier Science Publishing Co Inc
2. Principles of Biochemistry – A.L. Lehninger, D.L. Nelson and M.N. Cox, CBS Publishers and Distributors
3. Organic Synthesis – E.J. Corey and Xue Min Chen, Wiley, New York

Recommended Books:

1. Outlines of Biochemistry – E.E. Cohn and Stampf, Wiley Eastern
2. Modern Methods of Organic Synthesis – W Carruthers, Iain Coldham, Cambridge University Press

Course: Core 405 (PHYSICAL CHEMISTRY-IV)
Credit 4
Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To understand the concepts of dynamic electrochemistry, solid state electrochemistry, electrocapillary phenomenon, electrocatalysis and nanostructured and surface modified electrodes.
2. To impart knowledge on criteria and assumptions of non-equilibrium thermodynamics.
3. To understand the phenomenological equations and thermoelectric effects.

Expected Learner Outcome:

1. Students will gain knowledge in the thermodynamic and kinetic aspects of Electrochemistry through different fundamental concepts and models. They will also be able to solve problems in these areas.
2. Students will understand the concepts of uncompensated heat, microscopic reversibility, coupled reactions, thermoelectric effects.
3. Students will develop the skills to solve problems in non-equilibrium thermodynamics.

Unit I: Advanced Electrochemistry **Lecture 30, Marks 35**

Introduction to electrochemistry: Nernst equation, electrode kinetics, dynamic electrochemistry, the Butler-Volmer and Tafel equations. Overpotentials. Kinetically and mass transport controlled electrochemical processes. Mass transport by migration, convection and diffusion.Conductivity.Solid state electrochemistry.Ion conducting and electronically conducting polymers.The electrochemical double layer.Potentiostatic and galvanostatic electrochemical methods including chronoamperometry, coulometry, cyclic voltammetryandimpedance spectroscopy.

Thermodynamics of Electrocapillary phenomenon; Surface excess, relevance of outer and surface potential to double layer (DL) studies, surface and inner potential difference. Capacity potential relations in electrode-electrolyte interface, Contact adsorption-its influence on capacity of interface, Capacitance hump.

Electrocatalysis: Definitions, Electrocatalytic potential, effect of electric field on electrocatalysis,

Nanostructured and surface modified electrodes. Introduction to batteries, fuel cells and electrochemical solar cells. Electrochemical processes of particular relevance to energy conversion.

Unit II: Non-equilibrium Thermodynamics **Lecture 20, Marks 25**

Difference between equilibrium and non-equilibrium thermodynamics, Criteria of non-equilibrium thermodynamics; Assumptions of non-equilibrium thermodynamics, uncompensated heat and its relation to other thermodynamic functions, Fluxes and forces-relation between these two quantities, Entropy production in heat transfer, mass transfer in flow of current, in mixing of gases, and in chemical reaction;

The Phenomenological equations: The linear laws, The Onsagar relation, microscopic reversibility and Onsager reciprocity. Coupled reaction. Thermoelectric effects: Seebeck, Peltier and Thompson effect.

Text Books:

1. Modern Electrochemistry: Vol II by J. O. M Bockris & A. K. N. Reddy
2. Non Equilibrium Thermodymacis: Principles and application – C. Kalidas & M.V. Sangaranarayanan

Recommended Books:

1. Electrochemical Methods: Fundamentals and Applications, A. J. Bard, L. R. Faulkner, John Wiley and Sons.
2. Inorganic Electrochemistry: Theory, Practice and Applications by Piero Zanello
3. Non Equilibrium Thermodynamics by de Groot, S. R. and P. Mazur
4. Introduction to Thermodynamics of Irreversible Processes by I. Prigogine

Course: Core 406 (PHYSICAL CHEMISTRY-V)
Credit 4
Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
3	1	0	4

Objectives:

1. To introduce the Hartree Fock theory for treatment of atoms and molecules.
2. To lay the foundation of Density Functional Theory through historical developments and basic theorem.
3. To understand the applications of statistical thermodynamics on complex systems like classical liquids, phase transitions in lattice models etc.
4. To impart basic understanding of different simulation techniques.

Expected Learner Outcome:

1. Students will gain understanding of the advanced electronic structure of atoms/molecules through quantum mechanical methods, and will develop the skills to solve problems using those concepts.
2. Students will gain knowledge about modern day computational treatments of atoms and molecules and will understand applications of Density Functional Theory.
3. Students will be able to apply the concepts of statistical thermodynamics to understand complex systems and solve problems related to those systems.
4. Students will understand the theoretical background of different simulations techniques and there applicability to different problems.

Unit I:Advanced Quantum Chemistry **Lecture 26, Marks 30**

Antisymmetry Principle; Hartree product, Slater determinant; Slater-Condon rules; Hartree-Fock equations, Koopmans' and Brillouin's theorems, Roothaan equations, SCF procedure.
Computational treatment of atoms and molecules: Representation of molecules,Gaussian basis sets.
Introduction to Density functional Theory: Hohenberg-Kohn theorems; chemical concepts within the density functional theory.

Unit II: Advanced Statistical Mechanics **Lecture 24, Marks 30**

Classical Liquids Interparticle potentials, Configurational Partition functions, distributions, pair correlation function,radial distribution function, neutron scattering experiments, Virial equation, Meyer cluster diagrams.
Phase Transitions in Lattice models Lattice gas, Ising Model, order parameter, Mean Field theory, Renormalization group theory.
Computer Simulations Ensemble averages, ergodicity, random numbers, Monte Carlo methods, Molecular Dynamics, constant temperature MD.

Text Books:

1. Modern Quantum Theory – N. S. Ostlund and A. Szabo, McGraw Hill.
2. Statistical Mechanics – D.A. McQuarrie, Viva Books.

Recommended books:

1. Methods of Molecular Quantum mechanics, R. McWeeney and B. T. Sutcliffe, Academic Press.
2. Density functional theory of atoms and molecules, R. G. Parr and W. Yang, Oxford.
3. Introduction to Computational Chemistry by Frank Jensen
4. Essentials of Computational Chemistry: Theories and Models by C. J. Cramer
5. Molecular Modeling: Principles and Applications by A. R. Leach
6. An Introduction to Statistical Thermodynamics – T.L. Hill, Dover Books.
7. Statistical Mechanics – K. Huang, Wiley.
8. Statistical Thermodynamics – M.C. Gupta, Wiley Eastern Ltd.

Course: Core 407 (General Approaches to Research)
Credit 4
Total Marks 100 (End Semester 60 + Internal Assessment 40)

L	T	P	C
4	0	0	4

Objectives:
1. To understand the basic steps of a research process and to learn scientific data analysis.
2. To develop preliminary knowledge on the necessity of green chemistry practices.
3. To familiarize students with various greener approaches in chemical transformations.

Expected Learner Outcome:
1. Students will gain knowledge about the research process.
2. Students will develop the skill to analyze data in a scientific way.
3. Students will understand the importance of practicing green chemistry principles in synthetic laboratories.
4. Through this course they will develop skills to design greener methodologies for chemical transformations.

Unit I: Research Methodology **Lecture 20, Marks 30**

Meaning, objective and motivation of research, types of research, research methods versus research methodology, Research process, Defining and selecting a research problem, Literature survey (different sources of literature survey including online databases), defining hypothesis, Research design, Sampling Design, Data collection,
Data analysis: measures of central tendency, measures of dispersion, measures of asymmetry, measures of relationship. Regression analysis, t-test, p-test
citations and impact factors of journals, author index.

Unit II

A. Principles of Green Chemistry and Designing a Chemical synthesis:

Lectures 10, Marks 15

What is Green Chemistry? Need for Green Chemistry.Goals of Green Chemistry.Limitations?Obstacles in the pursuit of the goals of Green Chemistry; E-factor.
Twelve principles of Green Chemistry with their explanations and examples and special emphasis on the following:
i) Designing a green synthesis using these principles;Prevention of waste/ byproducts.
ii) Atom Economy, calculation of atom economy for chemical transformations.
iii) Prevention/ minimization of hazardous/ toxic products.
iv) Green solvents- supercritical fluids, water, ionic liquids and PEGs as green solvents for organic reactions.
v) Energy requirements for reactions- alternative sources of energy: use of microwaves and ultrasonic energy.
vi) Selection of starting materials; carbohydrates, CO_2, glycine betaine and vegetable oils as green starting materials.

vii) Use of catalytic reagents in preference to stoichiometric reagents; solid acids catalysis- use of zeolite, hydrotalcite etc. PTC catalyzed green reactions; co-enzymes as catalysts.Bioctalysis.Photocatalyzed reactions.
viii) Prevention of chemical accidents designing greener processes, inherent safer design.

B: Examples of Green Reagents/ Synthesis/ Reactions **Lectures 10, Marks 15**

(i) Green synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate, paracetamol, ibuprofen.
(ii) Microwave assisted reactions: Microwave assisted reactions in water (oxidation of toluene to benzoic acid, oxidation of alcohols); microwave assisted reactions in organic solvents (Diels-Alder reaction and Decarboxylation); Microwave assisted solvent-free reactions (solid state reaction)- Michael addition and Knoevenagel reaction)
(iii) Ultrasound assisted reactions: Grignard reaction, Ulmann coupling and Cannizaro reaction under sonication.
(iv) Dimethyl carbonate (DMC), Tetrabutylammoniumtribromide (TBATB) and Rongalaite as green reagents in organic synthesis.

Oxidation reagents and catalysts; Biomimetic multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions.Cocrystal Controlled Solid-State Synthesis (C^3S^3)

Text Books:

1. C. R. Kothari and Gaurav Garg, Research Methodology Methods andtechniques, New Age International
2. B. Saikia and D. Sarma, A textbook on Green Chemistry, Kalyani Publications (2017)

Reference Books:

1. P. T. Anastas& J. K. Warner: Oxford Green Theory and Practical, University Press (1998).
2. A. S. Matlack: Introduction to Green Chemistry, Marcel Dekker (2001).
3. M. C. Cann& M. E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
4. M. A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).

Course: DSE 408 (Project work)
Credit 8
Marks - 200 (End Semester 120 + Internal Assessment 80)

L	T	P	C
0	0	8	8

1. Research project approved by the Supervisor, preparation of the dissertation and presentationof the results and viva-voce examination by a board of examiners.

Dissertation	**Marks 90**
Viva-Voce	**Marks 30**