CENTRAL UNIVERSITY OF HIMACHAL PRADESH

Department of Chemistry and Chemical Sciences
School of Physical and Material Sciences

M.SC. CHEMISTRY SYLLABI

CENTRAL UNIVERSITY OF HIMACHAL PRADESH
[Established under the Central Universities Act 2009]
Dharamshala, District Kangra - 176215 (HP)
www.cuhimachal.ac.in

SEMESTER WISE COURSE STRUCTURE-DEPARTMENT OF CHEMISTRY-CUHP

Semester	Total Credits	Core Compulsory	Credits	Credits	Core Open		Credits
I	16	CCS 401- Organic Chemistry I	4				
		CCS 402 - Inorganic Chemistry I	4				
		CCS 403 - Physical Chemistry I	4				
		CCS 404 - Organic Chemistry Lab I	2				
		CCS 405 - Inorganic Chemistry Lab I	2				
II	14	CCS 406 - Physical Chemistry Lab I	2	2			
		CCS 407 - Organic Chemistry II	4				
		CCS 408 - Inorganic Chemistry II	4				
		CCS 409 - Physical Chemistry II	4				
III	4	Chemistry General-(Interdisciplinary topics)	4	6			
IV	6	M.Sc. Project	6	4	Computer applications in chemistry-I		4
					Computer applications in chemistry-II		4
Semester	**Total Credits**	**Elective specialization**		**Semester**	**Total Credits**	**Elective specialization**	**Credits**
III	8			IV	8		
		Advance Organic/Inorganic/Physical Chemistry Lab	2				
Semester	**Total Credits**	**Human Making & Skill Development courses**	2	**Semester**	**Credits**	**Elective Open**	**Credits**
I	4	HM -I	2	III	2		2
		SD- I	2				2
II	4	HM -II	2	IV	2		2
		SD- II	2				2

SEMESTER WISE COURSE STRUCTURE-DEPARTMENT OF CHEMISTRY-CUHP

SEMESTER	SUBJECT	CREDITS	TOTAL CREDITS
I	CORE COMPULSORY	16	20
	CORE OPEN	00	
	ELCTIVE SPECIALIZATION	00	
	HM+SD	04	
	ELECTIVE OPEN	00	
II	CORE COMPULSORY	14	20
	CORE OPEN	02	
	ELCTIVE SPECIALIZATION	00	
	HM+SD	04	
	ELECTIVE OPEN	00	
III	CORE COMPULSORY	04	20
	CORE OPEN	06	
	ELCTIVE SPECIALIZATION	08	
	HM+SD	00	
	ELECTIVE OPEN	02	
IV	CORE COMPULSORY	06	20
	CORE OPEN	04	
	ELCTIVE SPECIALIZATION	08	
	HM+SD	00	
	ELECTIVE OPEN	02	
TOTAL CREDITS			**80**

Proposed structure of courses to be offered in the Department of Chemistry and Chemical Sciences as per new Choice Bases Credit System (CBCS). A student needs to complete 80 credits to get Masters Degree.

CORE COMPULSORY COURSES

A student has to offer 40 credits from core compulsory courses				
Sr. No.	**Course Code**	**Course Name**	**Credits***	**Pre-requisite/ Remarks**
1	CCS 401	Organic Chemistry I	4	
2	CCS 402	Inorganic Chemistry I	4	
3	CCS 403	Physical Chemistry I	4	
4	CCS 404	Organic Chemistry Lab I	2	
5	CCS 405	Inorganic Chemistry Lab I	2	
6	CCS 406	Physical Chemistry Lab I	2	
7	CCS 407	Organic Chemistry II	4	
8	CCS 408	Inorganic Chemistry II	4	
9	CCS 409	Physical Chemistry II	4	
10	CCS 501	Chemistry General (Interdisciplinary Topics)	4	
11	CCS 565	M.Sc. Project	6	

**60 Lectures are recommended for 4 Credit courses & 30 Lectures are recommended for 2 Credit courses

CORE OPEN COURSES

A student has to offer 12 credits from core open courses				
Sr. No.	**Course Code**	**Course Name**	**Credits***	**Pre-requisite/ Remarks**
1.	CCS 410	Biophysical and Material Chemistry	2	
2.	CCS 411	Statistical error, electrochemical analyses, environmental analyses	2	
3.	CCS 412	Catalysis and green chemistry	2	
4.	CCS 413	Environmental chemistry	2	
5.	CCS 414	Chemistry of Xenobiotics Biodegradation-I	2	
6.				
7.	CCS 538	Biochemistry-I	2	
8.	CCS 539	Biochemistry-II	4	
9.	CCS 540	Advanced stereochemistry	2	
10.	CCS 541	Computer applications in chemistry-I	4	
11.	CCS 542	Computer applications in chemistry-II	4	

12.	CCS 543	Group theory and its applications in bonding	2	
13.	CCS 544	Structure and properties of solids	2	
14.	CCS 545	Chemistry of elements	2	
15.	CCS 546	Advanced bioinorganic chemistry	2	
16.	CCS 547	Biophysical chemistry	2	
17.	CCS 548	Data analysis & mathematical methods in chemistry	2	
18.	CCS 549	Electronic spectroscopy (absorption and emission)	2	
19.	CCS 550	Advanced statistical thermodynamics and symmetry	4	
20.	CCS 551	Physical methods of analysis and structure determination	4	
21.	CCS 552	Synthetic methodology & strategy	2	
22.	CCS 553	Chemoinformatics	2	
23.	CCS 554	Advance Bioorganic Chemistry	2	
24.	CCS 555	Advance Bio-Analytical techniques	2	
25.	CCS 556	Metabolomics and Biomarker study-I	2	
26.	CCS 557	Organic structure elucidation, characterization by spectrophotometry	2	
27.	CCS 558	Advance characterization techniques (FESEM,HRTEM, AFM, XRD)	4	
28.	CCS 570	Introduction to Medicinal Chemistry	2	
29.				
30.				
31.				

*60 Lectures are recommended for 4 Credit courses & 30 Lectures are recommended for 2 Credit courses

ELECTIVE SPECIALIZATION

(A student has to offer 16 credits from elective specialisation)
[CHOOSE 16 CREDITS FROM ANY ONE GROUP]

Note: A specialization shall only be offered if minimum 10 students have opted for it.

Specialization I: ORGANIC CHEMISTRY SPECIALIZATION				
Sr. No.	**Course Code**	**Course Name**	**Credits***	**Pre-requisite/ Remarks**
1	CCS 502	Organic Chemistry Specialization I	4	
2	CCS 503	Organic Chemistry Specialization II	4	
3	CCS 504	Organic Chemistry Specialization III	4	
4.	CCS 505	Organic Chemistry Specialization IV	4	
5.	CCS 506	Organic Chemistry Specialization V	2	

6.	CCS 507	Organic Chemistry Specialization VI	2	
7.	CCS 508	Organic Chemistry Specialization VII	2	
8.	CCS 509	Organic Chemistry Specialization VIII	2	
9.	CCS 510	Advance Organic Chemistry Lab I	2	
10.	CCS 511	Advance Organic Chemistry Lab II	2	
11.	CCS 512	Advance Organic Chemistry Lab III	2	
12.	CCS 513	Advance Organic Chemistry Lab IV	2	
13.	CCS 566	Special paper-I- Organic Chemistry	2	

Specialization II: INORGANIC CHEMISTRY SPECIALIZATION

Sr. No.	Course Code	Course Name	Credits	Pre-requisite/ Remarks
1	CCS 514	Inorganic Chemistry Specialization I	4	
2	CCS 515	Inorganic Chemistry Specialization II	4	
3	CCS 516	Inorganic Chemistry Specialization III	4	
4.	CCS 517	Inorganic Chemistry Specialization IV	4	
5.	CCS 518	Inorganic Chemistry Specialization V	2	
6.	CCS 519	Inorganic Chemistry Specialization VI	2	
7.	CCS 520	Inorganic Chemistry Specialization VII	2	
8.	CCS 521	Inorganic Chemistry Specialization VIII	2	
9.	CCS 522	Advance Inorganic Chemistry Lab I	2	
10.	CCS 523	Advance Inorganic Chemistry Lab II	2	
11.	CCS 524	Advance Inorganic Chemistry Lab III	2	
12.	CCS 525	Advance Inorganic Chemistry Lab IV	2	
13.	CCS 567	Special paper-II- Inorganic Chemistry	2	

Specialization III: PHYSICAL CHEMISTRY SPECIALIZATION

Sr. No.	Course Code	Course Name	Credits	Pre-requisite/ Remarks
1	CCS 526	Physical Chemistry Specialization I	4	
2	CCS 527	Physical Chemistry Specialization II	4	
3	CCS 528	Physical Chemistry Specialization III	4	
4.	CCS 529	Physical Chemistry Specialization IV	4	
5.	CCS 530	Physical Chemistry Specialization V	2	
6.	CCS 531	Physical Chemistry Specialization VI	2	
7.	CCS 532	Physical Chemistry Specialization VII	2	
8.	CCS 533	Physical Chemistry Specialization VIII	2	
9.	CCS 534	Advance Physical Chemistry Lab I	2	
10.	CCS 535	Advance Physical Chemistry Lab II	2	
11.	CCS 536	Advance Physical Chemistry Lab III	2	
12.	CCS 537	Advance Physical Chemistry Lab IV	2	
13.	CCS 568	Special paper-III- Physical Chemistry	2	
14.	CCS 569	Advance Practical course- (Organic + Inorganic + Physical)	2	

*60 Lectures are recommended for 4 Credit courses & 30 Lectures are recommended for 2 Credit courses

ELECTIVE OPEN COURSES

[For the students of the Department and students of other departments]

A students can offer 4 credits from this list of courses				
Sr. No.	**Course Code**	**Course Name**	**Credits**	**Pre-requisite/ Remarks**
1.	CCS 415	Green Chemistry and its application	2	
2.	CCS 416	Alchemy to modern Chemistry	2	
3.	CCS 417	Biosafety issues & Research ethics	2	
4.	CCS 418	Chemical data analysis	2	
5.	CCS 559	Advance Analytical techniques	2	
6.	CCS 560	Computational Chemistry	2	
7.	CCS 561	Food Chemistry	2	
8.	CCS 562	Clinical Chemistry	2	
9.	CCS 563	Chemistry of Organic materials	2	
10.	CCS 564	Assymatric organic synthesis/catalysis	2	
11.				
12.				
13.				
14.				
15.				

M.Phil & Ph.D. Courses:

Sr. No.	Course Code	Course Name	Credits	Pre-requisite/ Remarks
1.	CCS 599	Dissertation (M.Phil.)	20	
2.				
3.	CCS 601	Chemistry of Xenobiotics Biodegradation-II	6	
4.	CCS 602	Metabolomics and Biomarker study-II	6	
5.	CCS 603	Analytical Techniques in Metabolomics research	6	
6.	CCS 604	Microbial Metabolism for pollutant abatement-biochemical pathway analysis	6	
7.	CCS 699	Thesis (Ph.D.)	60	

Detail syllabus for the M.Sc. Chemistry course

[*Faculties can modify the content as per their convenience and requirement*]

CORE COMPULSORY

CCS 401- ORGANIC CHEMISTRY I [Credit -4]

UNIT-I: **Bonding in Organic Compounds-I**

Qualitative M.O. approach to bonding in organic molecules, Huckel`s rule and its applications to ethylene, cyclopentadiene, butadiene, cyclobutadine. Walsh orbitals of cyclopropane. Delocalized chemical bonding: conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerene, tautomerism. Huckel`s approach to conjugated systems, concept of aromaticity (η) in benzenoid and non benzenoid compounds, alternate and non-alternate hydrocarbons,. Energy level of pi–molecular orbitals;

UNIT-II: **Bonding in Organic Compounds-II**

Annulenes and heteroannulenes, fullerenes (C60), antiaromaticirty pseudo - aromaticity, homo aromaticity - PMO approach. Bonds weaker than covalent bond-addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catanates and rotaxanes. Stability of carbocations, strained organic molecules, calculation of strain energies.

UNIT-III: **Stereochemistry and Conformational Analyses**

Elements of symmetry, chirality, molecules with more than one chiral center, point groups, nomenclature: threo- and erythro- isomers, methods of resolution and optical purity, enantiotopic and diastereotropic atoms, groups and faces. Conformational analysis- acyclic systems up to 4 chiral centers, cyclohexane, cyclohexanone, cyclohexene; decalin, conformation of sugars. Effects of conformation on the reactivity of acyclic compounds and cyclohexanes. Stereochemistry of monocyclic, bicyclic and tricyclic systems (typical examples). Optical activity in absence of chiral carbon (biphenyls, allenes and spirans), chirality due to helical shape. Stereochemistry of organo nitrogen-, sulfur- and phosphorus-compounds.

UNIT-IV: **Organic Reaction Mechanism**

Addition to C-C multiple bonds : Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemo selectivity, orientation and reactivity. Hydrogenation of double and triple bonds and aromatic rings. Hydroboration reaction, Sharpless asymmetric epoxidation. Addition to Carbon- Hetero Multiple Bonds: Mechanism of metal hydride reaction of substituted and unsubstituted carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organo-Zn and organo-Li and organo Si reagents to saturated and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation involving enolates.

CCS 407-ORGANIC CHEMISTRY II [Credit -4]

UNIT I: **Pericyclic Reactions**

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3-buta diene, 1,3,5-hexatriene and allyl systems. Classification of pericyclic reactions. Woodward – Hoffmann correlation diagrams. FMO and PMO approach, concept of aromaticity of pericyclic transition states. Selection rules and stereochemical aspects of electrocyclic reactions, cycloaddition and sigmatropic shifts. Electrocyclic reactions: conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloaddition reactions: antarafacial and suprafacial additions, 4n and 4n+2 systems; 2,2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements: suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5-sigmatropic rearrangements. Sommelet-Hauser, Cope, Claisen, and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

UNIT II: **Heterocyclic Chemistry**

Systematic nomenclature (Hantzch-Widman system) for monocycle and fused heterocycles. General approaches to heterocycle synthesis – cyclisation and cycloaddition routes. Umpolung, synthon approach; Stork annulation reactions and recent applications (synthesis of testosterone, estrone, progesterone, ranitidine, lansoprazole and/or recently discovered molecules etc.); Rearrangement and ring transformation involving 5- and 6-membered heterocycles with one heteroatom.

UNIT III: **Chemistry of Natural Products-Ia**

Structural types; Biogenesis; Structure Elucidation and chemistry of representative examples of the following classes of natural products. *Alkaloids*- Structural types General introduction to phenylethylamine, pyrrolidine, pyridine, indole, isoquinoline type alkaloids. Structure elucidation (by chemical and spectroscopical methods), synthesis, biogenesis, biosynthesis, biological activity of atropine, nicotine, coniine and papaverine.

UNIT IV: **Chemistry of Natural Products-Ib**

*Terpenoid*s – Isoprene rule; structure elucidation (by chemical and spectroscopical methods), synthesis, biogenesis, biosynthesis of representative examples of acyclic, monocyclic and bicyclic monoterpenes. Structural types – general introduction to sesqui-, di-, and tri-terpenes.

CCS 402- INORGANIC CHEMISTRY I [Credit -4]

UNIT-I: **Aspects of Chemical Bonding**

LCAO-MO and VB treatments on H_2^+, H_2: Valence bond theory (VBT), resonance in VBT, VBT of homonuclear diatomic molecules, sigma and pi bonds, VBT of heteronuclear diatomic molecules, inadequacies of the simple VBT. Hybridization, participation of *d* orbitals in hybridization in polyatomic species. Molecular orbital theory (MOT), linear combination of atomic orbitals (LCAO), criteria for the formation of stable MOs. Sigma, Pi and Delta molecular orbitals. Homonuclear and heteronuclear diatomic molecules and ions. MO theory of polyatomic molecules and ions. MO theory of π bonding and multi-centre bonding. MO concept of metal-ligand bonding (pictorial approach); VSEPR Theory.

UNIT-II: **Theory of Coordination Chemistry-I**

Crystal Field Theory: Spitting of d orbitals in crystal fields of different symmetry for similar and dissimilar ligands (Octahedral, tetrahedral, Linear, trigonal planar, trigonal bipyramidal, square pyramid), crystal field stabilization energies (CFSE), spectrochemical series, octahedral site preference energy (OSPE) and their applications. Tetragonal distortion (John-Teller effect). Thermodynamic aspects of crystal field splitting (variation of ionic radii, lattice energy, hydration enthalpy and stability constants of complexes – Irving Williams order).

UNIT-III: **Theory of Coordination Chemistry-II**

Kinetic aspects of crystal field stabilization: crystal field activation energy, labile and inert complexes. Spin and orbital moments, spin-orbit coupling, quenching of orbital moment, spin only formula, temperature dependence of magnetic moment, Super exchange Phenomena, Diamagnetic Corrections. Dependence of Orbital contribution on the nature of the electronic ground state. Structural and stereoisomerism of coordination compounds, optically active coordination compounds and their resolution procedures, absolute configuration of enantiomers.

UNIT-IV: **Chemistry of d- and f- Block Elements (Comparative Study)**

Electronic configuration, oxidation states; aqueous, redox and complex chemistry, spectral and magnetic properties of compounds in different oxidation states, horizontal and vertical trends in respect of 3d,4d, and 5d elements with references to Ti-Zr- Hf , Cr- Mo- W, Mn Tc-Re and Pt group metals. Occurrence and isolation in respect of Mo, W, Re, Pt. Synthesis, properties, reactions, structure and bonding as applicable in respect of: Mo blue, W-blue, Pt-blue, W-bronze, Ru-red, Creutz- Traube complexes, Vaska`s complexes. Lanthanide and Actinide Elements; Nuclear stability, terrestrial abundance and distribution, relativistic effect, electronic configuration, oxidation states, aqueous-, redox and complex- chemistry; electronic spectra and magnetic properties (one example each). Lanthanide and actinide contractions and their consequences, separation of lanthanides and actinides and their applications (with examples).

CCS 408- INORGANIC CHEMISTRY II [Credit -4]

UNIT I: **Organometallic Chemisty-I**

The 18- electron rule for organometallic compounds of transition metals: Classification based on 18-electron rule: complexes of two, three, four, five six, seven, eight-electron pi-ligands: nomenclature. Exceptions to 18 electron rule: the 16-electron rule. Isolobal and isoelectronic relationship of complexes, Agostic interaction.
Metal-carbon-bonded compounds (compounds of the sigma electron ligands), Metal-alkyl, -allyl, -carbene, -carbonyl, -carbide and cyclopentadienyl complexes structure and bonding in η^2- ethylene and η^3- allylic compounds with typical examples, structure and bonding of $K[PtC_4H_4Cl_3]$, $[(Ph_3P)_2Pt(Ph\text{-}C{\equiv}C\text{-}Ph)]$, $[Co_2(CO)_6(Ph\text{-}C{\equiv}C\text{-}Ph)]$

UNIT II: **Organometallic Chemisty-II**

Elementary idea about homoleptic and non-homoleptic compounds: synthesis, reactivity, oxidative addition and reductive elimination reaction: insertion reactions and elimination; electrophilic and nucleophilic reactions; instability (decomposition pathway) and stabilization. Metallacycles.

UNIT III: **Molecular Clusters**

Main-group clusters: Geometric and electronic structure, three-, four- and higher connect clusters, the closo-, nido-, arachno-borane structural paradigm, styx No. of neutral and boron hydrides, Wade-Mingos and Jemmis electron counting rules, clusters with nuclearity 4-12 and beyond 12. Structure, synthesis and reactivity. Transition-metal clusters: Capping rules, metal-ligand complexes vs heteronuclear cluster. Main-group Transition-metal clusters: Isolobal analogs of p-block and d-block clusters, limitations and exceptions. Clusters having interstitial main group elements, cubane clusters and naked or Zintl clusters. Metal-carbonyl clusters, structures, capping and electron counting. Molecular clusters in catalysis, clusters to materials, boron-carbides and metal borides. [Lipscomb topological diagrams, polyhedral skeletal electron pair theory (PSEPT); Illustrative examples from recent literature-*not in details*].

UNIT IV: **Bioinorganic Chemistry**

Reversible oxygenation in life process O_2-uptake proteins, myoglobin, hemoglobin, hemeerythrin, hemocyanin and model systems, electron transport proteins, Fe-S proteins, ferridoxin, rubredoxin and model systems, respiratory electron transport chains: cytochromes, photosynthetic electron transport chain, chlorophyll, PS-I and PS-II, Biological nitrogen fixation (Nitrogenase) and abiological nitrogen fixation; metalloenzymes: – catalase, peroxidase, urease, superoxide dismutase (SOD), cytochrome P 450, cytochrome C oxidase, carbonic anhydrase, carboxypeptidase; molybdoenzymes.
Metal dependent diseases Wilsons, Alzheimer, vitamin B_{12} and B_{12} -enzyme, Metal complexes in therapeutic use of chelated and non chelated compounds, Chelation therapy.

CCS 403- PHYSICAL CHEMISTRY I [Credit -4]

UNIT-I: **Thermodynamics-I**

Classical Thermodynamics; Brief resume of the laws of thermodynamics, of concepts of enthalpy, free energy, chemical potential, entropies and spontaneity. Temperature and pressure dependence of thermodynamic quantities; Gibbs- Helmholtz equation. Chemical equilibrium: free energy and entropy of mixing. Partial molar properties: partial molar free energy, partial molar volume, partial molar heat content and their significances. Gibbs-Duhem equation. Maxwell's relations; elementary description of phase transitions; phase equilibria and phase rule; thermodynamics of ideal and non-ideal gases, and solutions.

UNIT-II: **Thermodynamics-II**

Statistical Thermodynamics; Thermodynamic probability and entropy, Maxwell Boltzman, Partition function: rotational, translational, vibrational and electronic partition functions of diatomic molecules, calculation of thermodynamic functions and equilibrium constants. Theories of heat capacities of solids. Concept of ensemble and ergodic hypothesis phase space. Microcanonical ensemble, Canonical ensemble distribution probability partition function, its relation with different thermodynamic state functions. Gibb's paradox and Sackur- Tetrode equation. Concept of thermal wave length. Equipartition theorem and its validity. Chemical potential and chemical equilibrium. Heat capacity of solids.

UNIT-III: **Surface Chemistry and dielectric Behaviour**

Surface phenomena: Vapour pressure over curved surface, the Young- Laplace equation, vapour pressure of droplets (Kelvin equation). The adsorption isotherms (Gibbs, Langmuir), BET equation, estimation of surface area. Surface active agents and their classification, Surface films on liquids, micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsion, reverse micelles. Study of surface phenomena by photoelectron spectroscopy, ESCA and Auger spectroscopy. Catalytic activity at surfaces.
Dielectric Behaviour: Dielectric polarization and solvent effect, polar molecules, Mossotti-Clausius relation and its limitations, Debye equation. Dipole moment and molecular structure. Intermolecular forces: attraction and repulsion potentials, van der Waals, Keesom, Debye and London forces and their relative contributions; Lennard-Jones potential. Hydrogen bonding. Onsager reaction field, dielectric effects on absorption and emission spectra. Lippert equation.

UNIT-IV: **Molecular spectroscopy, structure and properties**

Molecular spectroscopy: Introduction, elementary idea about spectroscopic instrumentation, spectral broadening. Electromagnetic spectrum and molecular processes associated with the regions. Rotational spectra of polyatomic molecules: classification of molecules into spherical, symmetric and asymmetric tops; linear triatomic molecules, Non-rigid rotor. Elementary idea of Stark effect. Anharmonic oscillator and dissociation. Elementary idea of Born-Oppenheimer approximation. Vibration rotation spectra for diatomic molecule, P-, Q-, R-branches of the vib-rotor spectrum. Rotational-vibrational coupling. Raman spectra: classical theory of Raman scattering, concept of polarizability ellipsoid. The 'Raman effect' and its salient experimental features. The classical and quantum explanation of the 'Raman effect'. Interpretation of Raman spectra of diatomic molecules.

CCS 409- PHYSICAL CHEMISTRY II [Credit -4]

UNIT I: **Quantum Mechanics**

Time independent Schrödinger equation, probability concept, concept of stationary state. Linear operators in quantum mechanics, Eigen value equation. Formal derivation of Heisenberg uncertainty principle: commutability and compatibility. Properties of the Hermitian operator, canonical commutation relations, Ehrenfest theorem. Applications: Particle-in-a box (1-, 2-, 3- dimensional), different potential functions and barrier problems, degeneracy, density of states. Simple harmonic oscillator: Ladder operator, properties of the

eigen functions. Rigid rotor: Angular momentum operator, spherical harmonics. Hydrogen atom: Details of the solution, shapes of the orbitals.
Approximate method: Elementary perturbation theory, Variation theorem, Simple applications.

UNIT II: **Atomic structure and Spectroscopy**

Motion under central force: Conservation of angular momentum and its consequence. Motion of angular momentum under magnetic field. Larmor prescision. Quantization rule and quantum numbers. Zeeman effect. Stern Gerlach experiment. Spin-orbit interaction, conservation of total angular momentum J, Vector atom model. Anomalous Zeeman effect, Paschen-Beck effect. Multielectron system- Pauli exclusion principle. Term symbols for simple multi-electron system. Magnetic moment and Lande's g factor. Schrödinger equation for hydrogen atom (only qualitative idea), separation of radial and angular part. Orbits and Orbitals. Shape of orbitals.

UNIT III: **Chemical Kinetics and Reaction Dynamics-I**

Reaction Dynamics: Rates and mechanisms of photochemical, chain and oscillatory reactions (hydrogen-bromine, hydrogen – chlorine reactions, pyrolysis of acetaldehyde, decomposition of ethane and Belousov- Zhabotinsky reaction as examples), dynamics of barrier less chemical reactions in solutions, dynamics of uni molecular reactions (Lindemann-Hinselwood and Rice-Ramsperger-Kasel-Marcus [RRKM] theories). Correlation between Kinetics and mechanism & vice-varsa. Enzyme catalysis; Michaelis-Menten equation

UNIT IV: **Chemical Kinetics and Reaction Dynamics-II**

Fast Ractions: Luminescence and energy transfer processes. Study of kinetics by stopped flow and relaxation methods, flash photolysis and magnetic resonance method. Statistical formulation of chemical kinetics reaction dynamics: Intermolecular collision and its consequence. Role of intermolecular potential, elastic and inelastic collision. Thermodynamics of reaction rates. Activation energy- Experimental and zero point activation energy. Rate constant expression for chemical reaction based on Eyring equation with examples. Physical rate processes –viscosity and diffusion.

CCS 501- CHEMISTRY GENERAL (INTERDISCIPLINARY TOPICS) [Credit -4]

UNIT I: **Supramolecular Chemistry**

Introduction, Origins and Concept. Molecular recognition. Host-guest complex. supramolecular orbitals, Supramolecular reactivity and catalysis. Self-assembly and self-organisation, Liquid crystals and supramolecuar polymers, polymer-surfactant interaction. supramolecular arrays: ribbon, ladder, rack, braded, grid; harnessing non-covalent forces to design functional materials; Definition, building block and spacer, molecular valency, noncovalent forces: pallet of hydrogen bondings, van der Waal interactions, pi-pi and C-H…pi interactions,

UNIT II: **Supramolecular Chemistry (Kinds and Characteristics)**

geometry setter, allosterism, proton and hydride sponges, principle of three C's, lock and key principle, Anion recognition and anion coordination chemistry. Different types of receptors with special reference of Crown ethers, cryptates and Calix[4]arene, superstructures in inorganic, metallo-organic, organometallic compounds, supramolecular devices, dendrimers. Application of supramolecular chemistry in drug design. Application in material science-molecular machines (Molecular sensors and supramolecular devices).

UNIT III: **Nanoscience and Technology**

Definition, historical perspective and effects of nanoscience and nanotechnology on various fields. Synthesis of nanoparticles by chemical routes and characterization techniques: Thermodynamics and kinetics of nucleation; Growth of polyhedral particles by surface reaction, Ostwald ripening, size distribution; TEM; SEM; AFM; Light scattering; XPS. Properties of nanostructured materials: Optical properties; magnetic properties; chemical properties. Overview of applied chemistry of Nanomaterials. Microporous materials, microgels, bioconjugate polymers, Nanoencapsulation.

UNIT IV: **Medicinal Chemistry**

Pharmakodynamics and pharmakokinetics and Drug design and synthesis of drugs, synthesis and chemistry of vitamins- vitamin-B complex, vitamin C, vitamin K. Drugs: Introduction, Classification of drugs, brief discussion of drug targets, Drugs based on enzyme inhibition: Sulfa drugs, penicillin antibiotics and fluorouracil (Mechanism of drug action). Drug targets on nucleic acids (Alkylating agents and intercalating agents). Definition of antagonist, agonist, prodrugs, pharmacokinetics and pharmacodynamics, concept of structure-activity relationship (SAR) and quantitative structure activity relationship (QSAR) with special reference to antimalarials, antibiotics, anticholenergics and CNS active drugs. Concepts of LD_{50} and ED_{50}, newer generation of antibiotics. Cardiovascular drugs, local anti-ionfective drugs.

CORE OPEN

CCS 410- BIOPHYSICAL AND MATERIAL CHEMISTRY- (Credit-2)

UNIT I: Structure of Biomolecules: Protein structure – building blocks, peptide bond, levels of structure; Biomolecular complexes: protein-ligand, enzyme-substrate.

UNIT II: Techniques for study of biomolecular structure and function- optical techniques: CD, ORD: Cotton effect, Faraday effect. Fluorescence anisotropy for biomolecular structure determination.

UNIT III: Classification of polymers, kinetics of two dimensional polymerization, condensation and addition polymerizations; initiation, propagation and termination; chain transfer, co-polymerization; molecular weight of polymers; determination of molecular weights.

UNIT IV: Statistics of Linear Polymer Chains: Polymer chain flexibility and internal rotation, random flight analysis of end-to end distance for freely jointed chain in one dimension and three dimensions. Effect of bond angle and restricted rotation on chain dimensions. Unperturbed chains. Long-range interactions and effect of solvent. Distribution of chain segments relative to centre of mass.

CCS 411- STATISTICAL ERROR, ELECTROCHEMICAL ANALYSES, ENVIRONMENTAL ANALYSES (Credit-2)

UNIT I: Errors in quantitative analyses, types of errors, handling of systematic errors, random errors, random walk phenomenon, Normal and Gaussian distribution and its properties, standard deviation, normal distribution of mean, confidence limits of the mean, propagation of random errors, presentation of results. Method of reporting computed data.

UNIT II: Toxic inorganic substances. Health hazards of SPM [Suspended (inorganic) Particulate Matter], IPM [Inhaleable (inorganic) Particulate Matter]. Methods of determination of SPM (High Volume Sampler) and IPM (Cascade Impactor). Heavy metal toxicities. Mechanism of toxicity. Pesticides, metallo-organic compounds and their toxicity. Application of some analytical methods to determine toxic species.

CCS 538- BIOCHEMISTRY-I (Credit-2)

UNIT I: Proteins: Classification, Amino acid, property, primary, secondary, tertiary and quaternary structure of protein. Determination of primary structure. Enzyme: Classification, nomenclature, Kinetic of enzyme action, comparative, uncooperative and non comparative inhibition, allo enzyme, isozymes.

UNIT III: Vitamins and Hormones: Fat soluble and water soluble vitamins .Vitamins as co enzymes and co-factor.NAD, FAD, TPP, Folic acid, Vit.B6, Vit.B2, Lipoic acid, Co ASH, Epinephrine, nor epinephrine, Steroid hormones.

UNIT III: Chemistry of lipids: Structure and function of bio membranes. Structure and function of lipids. Chemistry of carbohydrates: Classification and importance constitution plants and bacterial cell wall. Animal cell coat.

UNIT IV: Bioenergetics: The ATP cycle. Nucleic Acids: DNA and RNA. Type of RNA and their function. Property of DNA in solution. Watson - Crick Model of DNA structure. Replication, Transcription and translation, (in detail). Regulation of gene expression.

CCS 539- BIOCHEMISTRY-II (Credit-4)

UNIT I: **Carbohydrates and Lipids**: Conformation of monosaccharides, structure and functions of important derivatives of monosaccharides. N-acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides-starch and glycogen. Carbohydrate metabolism-Kreb's cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway. Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, lipoproteins-composition and function, role in atherosclerosis. Properties of lipid aggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membranes. Fluid mosaic model of membrane structure.

UNIT II: **Amino acids, Peptides, Proteins and Nucleic Acids**: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures. Α – helix, β-sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein- folding and domain structure. Quaternary structure. Amino acid metabolism- degradation and biosynthesis of amino acids, sequence determination: chemical/enzymatic/mass spectral, recemization/detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH). RNA and DNA Purine and pyrimidine bases of nucleic acids, base pairing via Hbonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code. Regulation of gene expression.

UNIT III: **Enzyme and Co-enzyme Chemistry**: Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic powder, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by use of inhibitors, affinity labeling and enzyme modification by site directed mutagenesis. reversible and irreversible inhibition. Transition-state, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortation. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A. Cofactors as derived from vitamins, coenzymes, prothetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid, vitamin B12. Mechanisms of reactions catalyzed by the above cofactors.

UNIT IV: **Organic Macromolecules**: Rise of the concept of polymers, general method of preparation, polymerization techniques, mechanistic understanding Polymer geometry, structural unit variety, and structural unit orientation. Synthesis and modifications of Macromolecules: Polylolefins, polystyrene and styrene copolymers poly vinyl chloride and related polymers, poly vinyl acetate. Acrylic fluoro polymers. Aliphatic polyethers. Polyamides, polyimides, polyesters, phenolformaldehyde polymers. Amino-polymers Polyurethanes, oxides. Polydienes rubbers. Modification in natural polymers such as cellulose and proteins.

CCS 540- ADVANCED STEREOCHEMISTRY- (Credit-2)

UNIT I: **Stereochemistry of polycyclic system:**
a) Conformation and reactivity of fused polycyclic systemsperhydrophenanthrenes, perhydroanthracene, steroids. b) Dynamic Aspects**:** Cyclisation reactions, Baldwin Rule; elimination, addition and rearrangement reactions.

UNIT II: **Chiroptic properties:** a) Optical activity**:** Principles, emperical rules and correlations, calculation of optical rotation. b) Optical rotatory dispersion (ORD)**:** Principles, cotton effects, empirical rulesaxial haloketone rule, octane rule, Lowe's rule, Determination of configuration and conformation. c) Circular dichorism (CD)**:** Principle, applications-determination of configuration, the exeiton chirality method; study of conformational changes, secondary structure of proteins.

CCS 541- COMPUTER APPLICATIONS IN CHEMISTRY-I - (Credit-4)

Introduction to programming languages; basic numerical analysis: solution of nonlinear equations using Newton-Raphson method (e.g. finding the roots of a cubic equation – vander Waals equation), solution of linear systems using Gaussian elimination, interpolation, numerical integration (trapezoidal and Simpson's 1/3rd rule), numerical solution of differential equations (Euler and Runge-Kutta method). Fourier transformations and applications in spectroscopy. Use of molecular geometry optimisation software (Gaussian 09); construction of z-matrix and concept of force field. Classical Molecular Dynamics (MD) simulation and application to simple systems like Lennard-Jones fluids. [Effort should be made to reproduce data reported in the literature using the above mentioned numerical methods wherever possible.]

CCS542- COMPUTER APPLICATIONS IN CHEMISTRY-II - (Credit-4)

1. Introduction to Linux operating system, basis Linux commands like Is, pwd, mkdir, cd, cp, mv, rm, cat, creating/editing a file etc.
2. Using a visualization software such as GNUPLOT: plotting (a) y=*x*, *x*2, sin *x* etc., (b) a data file.
3. Plotting of wavefunction and radial probability distribution of Hydrogen-like atoms.
4. Shapes of atomic orbitals and their visualisation.
5. Introduction to preliminary programming in FORTRAN with application in chemistry: Compiling and executing a programme, constants and variables, operations and symbols, expressions, airtmetic assignment, input/output statement, format statement, Do loop, conditions statement etc.

CCS 543- GROUP THEORY AND ITS APPLICATIONS IN BONDING (Credit-2)

UNIT I: Application of group theoretical methods for (i) construction of SALC's and their use in calculation of π MO's under the Huckel approximations, (ii) calculation of MO's of ABn type and sandwitch type molecules, (iii) study of hybridization. (iv) Conservation of orbital symmetry in pericyclic reactions.

UNIT II: Splitting of orbitals and free ion terms in weak crystal fields, symmetry and multiplicities of energy levels in strong crystal fields, correlation diagrams. Effect of lowering of symmetry on the orbitals and energy levels, correlation table.

CCS 544- STRUCTURE AND PROPERTIES OF SOLIDS (Credit-2)

UNIT I: Defects in solids, point, line and plane defects. Determination of equilibrium concentration of Schotky and Frenkel defects. Stoichiometric imbalance in crystals and non stoichiometric phases, color center in ionic crystals, band theory, band gap, metals and insulators, semiconductors, hoping semiconductors rectifiers and transistors, Bonding in metals; free electron theory, electronic specific heat, Hall effect, electrical and thermal conductivity of metals, superconductors; meissner effect, elementary concepts of BCS theory, ferroelectricity, antiferroelectricity, piezoelectricity, liquid crystals, cooperative magnetism.

UNIT II: Illustrative examples of ionic, covalent and hydrogen bonded solids; perovskite, ilmenite and rutile; spinel and inverse spinel, silicates: pyroxene, amphibole, talc, mica, clay, zeolite, ultramarine;

CCS 545- CHEMISTRY OF ELEMENTS (Credit-2)

UNIT I: Dinitrogen and dioxygen complexes, Iso- and heteropolyoxometalates with respect to V, Mo, and W: synthesis, reactions, structures, uses, Bonding in dirhenium complexes. Mixed valence compounds of Fe, Cu, Pt; Fe-S compounds, cobaloxime related compounds,

UNIT II: Conformational changes and thermochromism of Ni(II) compounds, Ru(II) and Ru(III) compounds, oxo compounds of Ru and Os, Rh(I) and Ir(I) carbonyl halide and carbonylhydrides.

CCS 546- ADVANCED BIOINORGANIC CHEMISTRY (Credit-2)

UNIT I: Bioenergetic principle and role of ATP, chemistry of respiration, DNA polymerization, metal ion interaction with nucleoside and nucleotide, metal ion transport and storage proteins, ferritin, transferrin, ceruloplasmin. Metal ion transport across biological membrane, enzymatic and ionophoric transport.

UNIT II: Study of metalloprotein and metalloenzyme: catalase, peroxidase, superoxide dismutase, ceruloplasmin, cytochrome oxidases, Ascorbate oxidase, Role of metal ions in different hydrolytic enzymes: Carbonic anhydrase, Carboxypeptidase, Urease, Toxic effects of metals and non metals. Specific examples of Pb, As, Hg, F.

CCS 547- BIOPHYSICAL CHEMISTRY (Credit-2)

UNIT I: The primary, secondary, tertiary and quaternary structures of proteins and enzymes. Function of proteins and enzymes. Nucleic acids: DNA, RNA, helix-coil transition, A, B and Z conformations. Free energy changes in biological reactions: ATP-ADP inter-conversion.

UNIT II: Biopolymer interactions – electrostatic, hydrophobic and dispersion forces. Multiple equilibria involving various types of binding processes. Thermodynamic aspects of biopolymer solutions – osmotic pressure, membrane equilibrium, muscular contraction, energy generation in mitochondrial system. Structures and functions of the cell membrane, ion-transport across biological membranes, muscle contraction and nerve function. Application of fluorescence spectroscopy in elucidating the structure and function of biomolecules.

CCS 548- DATA ANALYSIS & MATHEMATICAL METHODS IN CHEMISTRY (Credit-2)

UNIT I: Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

UNIT II: Solution of differential equations. Series solutions – Hermite, Legendre. Properties of special functions – gamma, delta functions.

UNIT III: Matrices and determinants. Vector calculus.

UNIT IV: Coordinate transformations. Legendre and Laplace transformations. Fourier analysis.

CCS 549- ELECTRONIC SPECTROSCOPY (ABSORPTION AND EMISSION) (Credit-2)

UNIT I: Qualitative treatment of Born-Oppenheimer separation, Frank-Condon principle, selection rules, characteristics of π-π^*, n-π^*, d-d transitions and their intensities. Apparent violation of selection rule (vibrational and spin-orbit couplings). Potential energy curves, mirror-image symmetry, deactivation – internal conversion and intersystem crossing, radiationless deactivation, fluorescence and phosphorescence.

UNIT II: Quenching of fluorescence, Life-time variation in presence of quencher. Excimers and exciplexes. Intermolecular energy transfer (FRET). Energy transfer and conformation distributions of biopolymers, protein fluorescence. Excited state proton transfer. Einstein theory – A, B coefficients, Principles of LASER and characteristic features.

CCS 550- ADVANCED STATISTICAL THERMODYNAMICS AND SYMMETRY (Credit-4)

UNIT-I: Brief revision of equilibrium thermodynamics, chemical equilibrium, Ideal and Real gases, ideal and non-ideal solutions. Non-equilibrium thermodynamics: Onsager reciprocity relations, entropy production and law of maximum entropy production.

UNIT-II: Statistical basis of thermodynamics, Concept of microstate and macrostate, Physical significance of number of microstates, Relation between statistical quantity (number of microstates) and thermodynamic quantities, Applications to Ideal monatomic gas Ensembles and postulates of statistical mechanics. Summary of thermodynamic results obtained for different ensembles.

UNIT-III: Boltzmann distribution for canonical ensembles. Applications of Canonical partition function to: Ideal monatomic gas Ideal diatomic and polyatomic gas Specific heats of solids. Grand Canonical partition function, Fermi-Dirac and Bose Einstein statistics.

UNIT-IV: Symmetry Significance of group theory and topology in chemistry. Group theory: Theory of representation. Reducible and irreducible representations. Construction of character tables. Complex characters. Direct product group and direct product representation. Symmetric direct product. Contact between group theory and quantum mechanics. The vanishing of integrals. Group-theoretical aspects of MO theories of structure and bonding of organic/inorganic molecules. Molecular geometry. Mulliken-Walsh diagrams for AH_2 molecules, the HOMO postulate. Huckel MOs for benzenoid systems. Isolobal mapping from organic to inorganic system. Selection rules for transition state. Selection rules for organic and inorganic reactions, using Woodward-Hoffmann and frontier-orbital (Fukui and Pearson) approach.

CCS 551- PHYSICAL METHODS OF ANALYSIS AND STRUCTURE DETERMINATION (Credit-4)

UNIT-I: **Mass Spectrometry**:

Theory of mass spectrometry, instrumentation, various types of ion sources, determination of molecular weight and molecular formula, metastable peaks. Typical fragmentation patterns of some functional group in organic molecules. Application of mass spectrometry in solving structural problems. Modern techniques used in Mass Spectrometry: Fast atom bombardment mass spectroscopy: Ion source for FAB and LSIMS. Ion formation in FAB, LSIMS, liquid matrices in FAB and LS, applications of FAB-MS. Matrix assisted laser desorption/ ionization: Ion formation, MALDI Matrices, sample preparation, application of MALDI, General characteristics of MALDI. Electrospray Ionisation: Development of ESI and related methods, ion source for ESI, ion formation in ESI, multiply charged ions, application of ESI-MS

Advanced Radio-Analytical Techniques
Proton induced X-ray Emission and applications, Nuclear Activation analysis and applications, Solid State, Nuclear Track Detection and applications.

UNIT-II: **Supramolecular structures and their determination**:

Introduction to supramolecular chemistry and supramolecular structures-basics and concepts. Non-covalent interactions in supermolecules; their nature type and role in pre- organization and complementarity. Introduction to supramolecular synthons. Anion binding sites and anon receptors.

Electrochromatography:
Electrophoresis, Basic principle and types, Slab and Capillary electrophoresis, Instrumentation and applications of Capillary Electrophoresis, Capillary Zone Electrophoresis of small ions and molecular species, Capillary Gel Electrophoresis in DNA sequencing, Capillary Isotachophoresis, Capillary Isoelectric Focusing, Micellar Electrokinetic chromatography, packed column electrochromatography. Supramolecular reactivity and catalysis. Applications of supramolecular chemistryintroduction to molecular devices.

UNIT-III: **X-ray Crystallography**

X-RAYS, CRYSTALS AND GEOMETRIC DATA COLLECTION: Use of X-ray diffraction to find atomic arrangements. Point group, space group and unit cell. Concept of reciprocal lattice. Bragg law in reciprocal space. COMBINING WAVES TO OBTAIN AN IMAGE: Elementary treatment of Structure factor and Fourier synthesis. Anomalous scattering and its effects. CRYSTALS AND INTESITY DATA COLLECTION: Fundamental concepts. THE PHASE PROBLEM IN CRYSTALLOGRAPHY: Direct methods of relative phase determination. Patterson method and heavy atom method. R-Factor criterion. Structure completion in practice. REFINEMENT OF CRYSTAL STRUCTURE: Mention of refinement by Fourier synthesis. The method of least squares. Goodness of fit parameter, weighting functions. DERIVED RESULTS AND APPLICATIONS: Representation of structural results. Chirality and absolute structure. Packing in crystals. Thermal and Photochemical reactions in solid state. Topochemical principle. Topotactic reactions. Conformation of polypeptides: Ramachandran plot.

UNIT-IV: **Solids State and Advanced Materials**

(a) Dislocations in solids, schottky and Frenkel defects, defects, defect concentration. Band theory of solids, significance of band gap, conductors, semi-conductors and insulators. (b) Electrical & optical properties: Electrical conduction in metals, superconductivity, meisner effect, origin of superconductivity. Dielectric polarisation, ferroelectric and piezo-electric materials. (c) Magnetic properties: Origin of magnetic dipoles in solids. Paramagnetic spin systems, spontaneous magnetization, ferrimagnetic materials, Quantum Hall Effect (d) Solid Surface: Determination of surface structure by LEED techniques photoelectron Spectroscopy (ESCA) and Auger Spectroscopy. (e) Processing of Materials using Gamma rays and Electrons, Swift Heavy Ion Modified Material.

CCS 552- SYNTHETIC METHODOLOGY & STRATEGY (Credit-2)

UNIT I: Synthetic methodology: The roles of boron, phosphorus, sulfur and silicon in organic synthesis. Stereoselective hydroboration, hydrogenation, epoxidation and hydroxylation.

UNIT II: Synthetic strategy: Retrosynthetic analysis, disconnection, typical examples to illustrate the disconnection approach to organic synthesis.

UNIT III: Polimerisation Reactions: monomers, dimmers and oligomers, polymerization by-carbonyl substitution reactions, electrophilic aromatic substitution reactions,

UNIT IV: SN2 reactions, nucleophilic attack on isocyanates; polymerizations of alkenes, co-polymerisation, crossedlinked polymers, biodegradable polymers and plastics.

PRACTICALS

CCS 404- LIST OF ORGANIC CHEMISTRY PRACTICALS (Credit-2)

Faculty can choose as per convenience

Experiment-1: Chemical separation of organic compounds and Identification.

Experiment-2: Separation, purification and identification of organic compounds in binary mixtures (two solids, one solid + one liquid) using TLC, PC, column chromatography, chemical tests, UV-, IR- spectral measurements as required.

Experiment-3: Preparation of organic compounds by typical organic reactions, purification and characterization of the product [by re-crystallization, TLC, PC, determination of R_f value as required, m.p/b.p. , UV, IR spectra (as applicable)]:

SET I:

Oxidation: Adipic acid from cyclohexanol (by chromic acid oxidation).

Grignard reaction: Triphenylcarbinol from benzoic acid.

Aldol condensation: Dibenzal acetone from acetone and benzaldehyde.

Sandmeyer reaction: p-Chlorotoluene from p- toluidine.

Cannizzro reaction: Using p chlorobenzaldehyde as the substrate.

Fridel-Craft reaction: β-Benzoylpropeonic acid from succinic anhydride and benzene.

Acetoacetic ester condensation: Ethyl n butylacetoacetate from ethylacetoacetate.

Aromatic electrophilic substitution: p Nitroaniline from p-bromoaniline.

Parkin reaction: Cinnamic acid from benzalehyde and potassium acetate.

SET II:

1. *Oxidation* of benzylic carbon by prior protection of $-NH_2$ group in the nucleus followed by deprotection: 4-Aminotoluene ---- 4-Aminobenzoic acid

2. *Preparation of imide* followed by *Hofmann degradation*: Phthalic anhydride ---- Anthranilic acid

3. *Reductive removal* of aromatic amino group by prior diazotization followed by *Sandmeyer reaction*: Anthranilic acid ---- o Chlorobenzoic acid.

4. *Nitration* of aromatic ester followed by hydrolysis: Methylbenzoate -------- 3-Nitrobenzoic acid

5. *Oxidation* of α–hydroxyketone to diketone followed by rearrangement: Benzoin ------ Benzilic acid.

6. *1,4-Dihydropyridine ring generation*: Ethyl acetoacetate -------- 2,6-Dimethyl-3,5-dicarbethoxy-1,4-dihydropyridine.

7. *Partial reduction* of aromatic dinitro compound: m-Dinitrobenzene ------- m-Nitroaniline.

8. *Benzoylation* of amino group in presence of carboxylic acid group: Glycine ------ Hippuric acid.

9. *Reduction* of a hydroxycarboxylic acid with HI and red P: Benzilic acid--------- Diphenylacetic acid.

CCS 405- LIST OF INORGANIC CHEMISTRY PRACTICALS (Credit-2)

Faculty can choose as per convenience

Experiment-1: Spectrophotometric Estimations:

(i) Fe^{III} as $[Fe^{III}(SCN)^{2+}]$ complex (ii) Mn as MnO_4^- (iii) Phosphate as phosphomolybdate blue complex (iv) Fe^{III} and Fe^{II} in mixture as $[Fe^{II}$ (1,10-phenanthroline)$_3^{2+}]$ complex (v) $Cr_2O_7^{2-}$ and MnO_4^- in mixture (vi). Ti^{IV} and V^{v} in mixture as their H_2O_2 complexes (vii). Cu^{II} and Zn^{II} as their PAR complexes.

Estimations based on ion-exchange separation, acid base, complexometric and argentimetric titrations. Hardness of water, separation of (i) Zn^{II} + Mg^{II} (ii) Cl^- + Br^- mixtures (iii) Co^{II} + Ni^{II} (iv) Zn^{II} + Cd^{II} (v) K^+ : H^+ : SO_4^{2-} ratio in $KHSO_4$ (vi) H^+ , Na^+, Mg^{2+} and Zn^{2+} in mixture (vii) Al^{3+}, Fe^{3+}, Co^{2+} and Ni^{2+} in mixture.

Experiment-2: Semi-Micro Qualitative Inorganic Analysis of Complex Inorganic Mixtures containing not more than six (6) inorganic radicals from the lists : (a) Cation Radicals derived from: Pb, Bi, Cu, Sb, Sn, Fe, Al, Cr, Co, Ni, Mn, Zn, Ba, Sr, Ca, Mg, Na, K and NH^{4+} ion. (b) Anion Radicals: F^-, Cl^-, Br^-, I^-, BrO_3^- , IO_3^-, SCN^-, S^{2-}, $S_2O_3^{2-}$,SO_3^{2-}, SO_4^{2-}, NO_2^-, NO_3^-, PO_4^{3-}, BO_3^{3-}, H_3BO_3, SiO^{2-},CrO_4^{2-}, $Cr_2O_7^{2-}$, $[Fe(CN)_6^{4-}]$, $[Fe(CN)_6^{3-}]$. (c) Insoluble Materials: $PbSO_4$, $BaSO_4$, $SrSO_4$, $PbCrO_4$, CaF_2, SiO_2 and various silicates, SnO_2, Al_2O_3, Fe_2O_3, Cr_2O_3, AgCl, AgBr, AgI. (d) Cation radicals, anion radicals and insoluble materials derived from the following rare Elements: V, Mo, W, U, Ti, Zr, Ce, Th and Be.

Experiment-3: 1. Determination of the amount of calcium in milk powder by EDTA complexometry

2. Potassium trioxaltoferrate III: Sythesis, analysis and photochemistry.

3. Analysis of kidney stones by permanganometric titration

4. Preparation of $[Ni(NH_3)_6]^{2+}$ and its analysis by different methods

5. Estimation of iodine in iodized common salt using iodometry

6. Estimation of phosphoric acid in cola drinks by molybdenum blue method

7. Paper and column chromatography of plant pigments

CCS 406- LIST OF PHYSICAL CHEMISTRY PRACTICALS (Credit-2)

Faculty can choose as per convenience

SET I:

1. Spectrophotometric experiment - determination of composition of a complex (Job's method)

2. Determination of cmc of surfactants: conductometry and spectrophotometry.

3. Determination of molecular weight of macromolecules by viscometry.

4. Determination of dipole moment.

5. Analytical experiments: Study of distribution of an organic acid in an organic solvent and water – determination of association constant (with the help of Nernst distribution law), determination of van't Hoff factor.

6. Determination of transport number.

7. Molecular structure determination – gas phase vibrational rotational spectra of HCl/DCl.

SET II:

(A) Conductometry: 1. Determination of strengths of strong and weak acids in a mixture conductometrically

2. Determination of strengths of halides in a mixture conductometrically by precipitation titrations

3. Determination of concentrations of halides and halogen acids in a mixture conductometrically by precipitation titrations (system: HCl + KCl mixture by titration with standard NaOH and standard $AgNO_3$ solutions

4. Verification of Ostwald's dilution law conductometrically

5. Determination of critical micelle concentration (CMC) of a surfactant by conductometric method

(B) Potentiometry / pH-metry: 6. Determination of strengths of strong and weak acids in a mixture potentiometrically / pH-metrically (system: acetic acid + HCl)

7. Determination E° value of redox couples (i). Quinhydrone electrode (ii). Ferricyanide-ferrocyanide couple (iii). AgCl/Ag electrode

8. Determination of strengths of halides in a mixture potentiometrically by precipitation titrations (0.02N KBr + 0.02N KI mixture with standard 0.1N $AgNO_3$)

9. Determination of concentration by potentiometric / pH- metric titrations: (i). Acid-base titration (standard oxalic acid vs. NaOH, acetic acid vs. NaOH) (ii). Determination of ferrocyanide ion using standard bromate solution (iii). Determination of iodide ion by differential redox titration using standard bromated solution (iv) Determination of composition of zinc-ferrocyanide complex by potntiometric titration

(C) Colourimetry: 10. Determination of pKa of an indicator by colourimetric method (systems: methyl red, methyl orange, alizarin red –S in aqueous solution)

11. Kinetic studies on iodination of aniline (d) Polarimetry:

12. Determination of specific rotation and molar rotation of dextro-tartaric acid

13. Polarimetric determination of rate constant of reactions: (i). Inversion of sucrose (ii). Mutarotation of glucose (determination catalytic coefficients: k_{H+} and k_{H2O})

SET III:

Group-a: Phase-rule; 1. Determination of critical solution temperature (system: phenol water)

2. To construct the phase diagram of a three component system: (i).Chloroform acetic acid-water (ii). Benzene-acetic acid-water (iii). Nitrobenzene-acetic acid-water

Group-b: Adsorption; 3. To study the surface tension – concentration relationship of solutions (Gibbs equation)

Group-c: Kinetics; 4. Determination of rate constant of reactions: (i). Iodination of acetone (zero order) (ii). Decomposition of H_2O_2 (first order) (iii). Oxidation of iodide ion by bromate ion (second order)

5. Determination of rate constant of oxidation of iodide by H_2O_2 and to study the kinetics of iodine-clock reaction

Group-d: Thermodynamics & Equlibrium; 6. Determination of exchange capacities of ion-exchange resins and studies on ion-exchange equilibria.

7. Determination of solubility and solubility product of salts (systems: PbI_2, Potassium hydrogen tartarate)

8. Determination of partition coefficients of a solute between two immiscible solvents (systems: benzoic acid between benzene and water)

9. Determination of composition of complexes formed in solution (systems: Cu^{2+} - NH_3, Ag^+ - NH_3).

10. Determination of equilibrium constant of hydrolysis of an ester.

11. Determination of isoelectric point by viscosity measurement

CHEMISTRY SPECIAL PAPERS

CCS 502- ORGANIC CHEMISTRY SPECIALIZATION I (Credit-4)

UNIT I: **Advanced Organic Syntheses-I**

Common named reactions and rearrangements – applications in organic syntheses. Organic transformations and reagents: Functional group interconversion including oxidations and reductions; common catalysts and reagents (organic, inorganic, organometallic and enzymatic). Chemo, regio and stereoselective transformations. Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups. One group - C-X and two groups C-X disconnections; One group C–C and two group C–C disconnections (typical examples), use of acetylenes and aliphatic nitro compounds in organic synthesis. Diels-Alder reactions, 1,3- and 1,5- di-functionalised compounds, β,α-unsaturated carbonyl compounds, control in carbonyl condensation, Michael addition and Robinson annealation. Ring synthesis: saturated heterocycles synthesis of 3-, 4-, 5-, and 6-membered rings, aromatic heterocycles in organic synthesis.

UNIT II: **Advanced Organic Syntheses-II**

Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction –substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio discrimination. Resolution – optical and kinetic.

UNIT III: **Chemistry of natural Products-II**

Stereochemistry, reaction and biosynthesis of *terpenoid*s and *carotenoids*: zingiberine, santonin, abietic acid, β-carotene. Stereochemistry, reactions and synthesis of *alkaloids*; quinine, morphine, camptothecin. Structure, biosynthesis and reactions of *flavonoids* and coumarins. Reaction and biosynthesis of *steroids*: cholesterol, bile acid, testosterone, estrone, progesterone. Structure and biosynthesis of *porphyrins*: haemoglobin, chlorophyll. Structure and synthesis of *prostaglandins*: PGE_2, $PGF_{2\alpha}$. Shikimic acid pathway.

CCS 503- ORGANIC CHEMISTRY SPECIALIZATION II [Credit-4]

UNIT I: **Mass spectrometry**

Basic instrumentation, ion production - E1, C1, FD, FAB and MALDI techniques. Mass spectral fragmentation of typical organic compounds, common functional groups.

UNIT II: **Nuclear Magnetic Resonance (NMR) Spectroscopy**

Basic instrumentation, nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J'- Karplus equation. Classification of molecules. (AB, ABX, AMX, ABC, A_2B_2 etc. types), spin decoupling. FT NMR. (qualitative idea) and its advantages.

UNIT III: **Techniques of Chemical Separation**

Principles, classification, experimental set up, special features, mechanism of separation procedures, advantages and disadvantages, and applications (analytical and/or industrial) of the following separation techniques.

i. **Chromatography :** Fundamentals, dynamics, plate theory, resolution of mixtures. Absorption chromatography-chemical constitution and chromatographic-behaviour, affinity chromatography and chiral chromatography. Partition chromatography-liquid liquid and reverse phase partition chromatography, paper chromatography, thin layer chromatography (TLC) and ion pair chromatography. HPLC.
ii. **Gas chromatography (GC) :** Plate theory, gas-solid and gas-liquid chromatography. Super critical fluid chromatography, gel permeation chromatography and molecular sieves. Hyphened technique. GC-MS and its applications.
iii. **Electrochromatographic techniques :** Curtain electro-chromatography, reverse osmosis and electro-dialysis and their applications in desalination of water, separation of biomolecules by electrophoresis, capillary electrophoresis.
iv. **Solvent extraction :** Extraction equilibria, partition coefficient and extraction coefficient, extraction by chelation and solvation; solid-phase extraction (SPE), supramolecular extraction with crown ethers, cryptands and rotaxenes.

UNIT IV: **Green Chemistry**

Twelve principles of Green Chemistry, Green synthetic methods, catalytic methods, organic synthesis in aqueous media, Ionic liquid, supercritical fluids and microwave. Solvent-free organic reactions.

CCS 504- ORGANIC CHEMISTRY SPECIALIZATION III [Credit-4]

UNIT I: **Organometallic Chemistry of Transitional Elements**

Preparative structural and characteristic aspects. Bonding of hydrocarbon ligands, metallocenes, oxidative insertion, reductive elimination, ligand migration from metal to carbon; organometallics as electrophiles. Davies rules, catalytic nucleophilic addition and substitution, coupling reactions, Heck, Suzuki and Stille reactions, hydrogenation hydroformylation, carbonylation of methanol, oxidations, alkene polymerisation, Ziegler-Natta reaction, olefin metathesis, Tebbe's reagent, Pauson-Khand reaction, Volhardt cotrimerisation. Fluctional organometallic compounds. Chemistry and use of organo-derivatives of non-transitional metals- tin, thalium, mercury, lead.

UNIT II: **Synthetic Methodology II**

Organophosphorus compounds-Chemistry of organophosphorus compounds, phosphorus ylids and chiral phosphines.

Organosulphur compounds-Chemistry of organo sulphur compounds, sulphur stabilized anions and cations, sulphonium salts, sulphonium and sulphoxonium ylids, chiral sulphoxide.

Organosilicon compounds - Synthetic uses of silyl ethers, silylenol ethers, TMSCl, TMSI, TMSCN, alkene synthesis, alkynyl, vinyl, aryl, allyl and acylsilanes; Brook rearrangement, silicon Baeyer Villiger rearrangement

UNIT III: **Advanced Pericyclic Reactions**

General perturbation molecular orbital theory in cycloadditions : Reactivity, regioselectivity and periselectivity. Cheletropic reactions, 1,3-dipolar cycloadditions, cycloaddition involving more than 6 electrons, charged species, three-component and four component cycloadditions. Ene reactions, group-transfer reactions and eliminations. Electrocyclic reactions of charged systems (cations and anions) Sigmatropic rearrangements : [1,j] shifts-[1,5] and [1,7] carbon shifts in neutral systems and [1,4] shifts in charged species : [i,j] shifts- [3,3] shifts, fluctional molecules; [5,5] shifts, [2,3] shifts in ylids.

CCS 505- ORGANIC CHEMISTRY SPECIALIZATION IV (Credit-4)

UNIT I: **Dynamic Aspects of Stereochemistry**

Stereoselective and stereospecific synthesis, enantio- and diastereo-selective synthesis; n-facial selectivity, Cieplak model, carbohydrates as chiral pool material. Diastereoselective reactions **:** Addition to prochiral and chiral carbonyl compounds, reactions of chiral enolates; α-substitution of prochiral ketones (RAMP/SAMP and related methodologies); aldol reactions, addition to C=C bonds, conjugated addition. Enantioselective reactions : Chiral catalysis sharpless epoxidation and dihydroxylation; asymmetric cyclopropanation; asymmetric hydrogenation, CBS reduction; Baker's yeast mediated reduction; enzyme mediated hydrolysis and esterification of meso compounds. Enantioselective synthesis.

UNIT II: **Advance Heterocyclic Chemistry**

Synthesis, reactions and their mechanisms of aziridine, azetidine; pyrazines and their analogues; oxazole, thiazole, imidazole, iso-oxazole, isothiazole and corresponding fused systems; pteridines, folic acid. Nomenclature of bicyclic and tricyclic fused system. Introduction to chemistry of azepins, oxepins, thiepins and their aza analogues; phosphorous-containing and selenium containing heterocycles.
ANRORC and Vicarious nucleophilic substitutions in heterocycles.

UNIT III: **Organometallic Reagents in organic syntheses and Structure Determination of Organic Compounds**

(a) Use of Si, S, B, Cr, Ti, Co, Rh, Ru, Pd, Cu, Ni, Fe and Ce in organic syntheses.
(b) Elucidation of the structures of the organic molecules by spectra (IR, UV-vis, NMR and Mass)

CCS 506- ORGANIC CHEMISTRY SPECIALIZATION V (Credit-2)

Oxidation and Reduction of Functional Groups

UNIT I: **Oxidation reactions:** Oxidation of hydrocarbons, oxidation of alcohols by various reagents, and methods, oxidation of carbon-carbon double bonds to diols and epoxides, Woodward and Prevost Reaction, synthetic reactions of epoxides, diastereo-selective epoxidation of homoallylic alcohols, photosensetised oxidation of alkenes, oxidation of ketones to αβ- unsaturated ketones. Oxidation with ruthenium tetroxide, iodobenzene diacetate, and thallium (III) nitrate.

UNIT II: **Reduction reactions:** Catalytic hydrogenation-the catalyst, selectivity of reduction, reduction of functional groups,stereochemistry and mechanism, homogeneous hydrogenation. Reduction by dissolving metals-reduction with metal and acid, reduction of carbonyl compounds, Birch Reduction. Reduction by hydride transfer reagents-aluminium alkoxides, LAH and $NaBH_4$, lithiumhydridoalkoxyaluminates, lithiumaluminiumhydride aluminiumchloride reagents, diisobutylaluminiumhydride, sodiumcyanoborodydride, trialkylborohydrides. Other methods-desulphurisation of thio-acetals, di-imides, low-valent titanium species, trialkyltinhydrides.

CCS 507- ORGANIC CHEMISTRY SPECIALIZATION VI (Credit-2)

Photo Organic Chemistry and Free Radical Reactions

UNIT I: **Photo Organic Chemistry:** Basic principles, Jablonsky diagram, exciplex, photochemistry of alkenes-intramolecular reactions of olefinic bond- geometrical isomerism, cyclization reactions, rearrangements of 1,4 and 1,5 dienes. Photochemistry of carbonyl compounds intramolecular reactions of saturated-, cyclic- and acyclic-, α,β-unsaturated- and γ,β-unsaturated carbonyl compounds, cyclohexadienones. Intramolecular cycloaddition reaction dimerization and oxetane formation. Norrish type I and type II reactions, di-pi-methane rearrangements. Photochemistry of aromatic compounds : isomerisation, addition and substitution reactions. Miscellaneous photochemical reactions. Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction.

UNIT II: **Free Radical Reactions**: a) Methods of generation and detection of free radicals (trapping, ESR, NMR- CIDNP). b) Reactivity pattern of radicals, substitution and addition reactions, neighbouring group assistance. Reactivity of typical aromatic and aliphatic substractes at a bridge head, the effect of solvent on reactivity, oxidation of aldehydes to carboxylic acids, autooxidation, coupling of alkynes. Radical rearrangement. c) Radical cations and radical anions, single electron transfer reactions, SRN1 reactions.

CCS 508- ORGANIC CHEMISTRY SPECIALIZATION VII (Credit-2)

Advance Spectroscopy

UNIT I: **Review of UV and IR spectroscopy**

UNIT II: **Nuclear Magnetic Resonance (NMR) spectroscopy:** Chemical shift values and correlation of protons bonded to carbon atom in aliphatic, olefinic, aromatic compounds, alcohols, aldehydes, phenols, enols, carboxylic acids, amines, amides and mercaptans; chemical exchange: effect of deutaration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique (FT-NMR), nuclear overhauser effect (NOE), ^{19}F and ^{31}P NMR (examples).

UNIT III: **Carbon-13 NMR spectroscopy**: Chemical shifts(additive shift parameters in alkanes, alkenes, cyclohexane and its derivatives, benzenoid systems) for aliphatic alkenes, alkyne, aromatics, hetero- aromatics and carbonyl carbon atoms, coupling constants. Two dimensional NMR spectroscopy-COSY (1H-1H correlation), NOESY, DEPT, INEPT, APT, HMQC (heteronuclear multi-quantum coherence, 1-bond ^{1}H-^{13}C correlation) HMBC and INADEQAUATE techniques. Pulse sequences of various 2D NMR spectroscopic techniques.

CCS 509- ORGANIC CHEMISTRY SPECIALIZATION VIII (Credit-2)

UNIT I: **Chemistry of Medicinally Important Molecules**

Bacterial and animal cells, antibacterial agents – mechanism with reference to β-lactam antibiotics; General method of synthesis of β-lactam ring: synthesis of penicillin, 6-APA, cephalosporin, 7-ACA; Morin – Jackson rearrangement; Structure-activity relationship of penicillin. New generation antibiotics / antibacterial agents: Synthesis and mechanism of action of (i) fluoroquinolones – norfloxacin, ciprofloxacin, levofloxacin (ii) anti AIDS drugs – AZT, lamivadine (iii) antihypertensive agent – captopril (iv) calcium channel blocker – amlodipine (v) gastric secretion inhibitor – omeprazole (vi) drug for impotency – sildenafil etc.

UNIT II: **Synthetic methodology and strategy for few compounds:**

(i) cationic cyclisations: progesterone (Johnson) (ii) radical cyclisations: synthesis of hirsutene (Curran) (iii) pericyclic reactions: endiandric acids (Nicolaou); (iv) Photochemical reactions: strained compounds (isocomene by Pirrung) (v) aldol reactions: Prelog-Djerassi lactone; (vi) carbene reactions: making cyclopropanes (vii) biomimetic strategy: carpanone (Chapman) (viii) solidsupported reagents, solid phase synthesis: plicamine (Ley) (ix) combinatorial synthesis etc.

CCS 514- INORGANIC CHEMISTRY SPECIALIZATION I (Credit-4)

UNIT I: **Group theory and its Applications in Spectroscopy**

The Great Orthogonality Theorem: statement and interpretation, proof of important corollaries; construction of character tables, cyclic groups and construction of their character tables, direct product groups and construction of their character tables, direct product representations. Application of group theoretical methods for (i) selection rules, allowedness/forbiddenness of n-π* and π-π* transitions, (ii) splitting of terms in octahedral and tetrahedral ligand fields, Orgel and Tanabe-Sugano diagrams, (iii) symmetry aspects of molecular vibrations,justification of Laporte selection rule, vibronic coupling and vibronic polarization of electronically allowed transitions, infrared and Raman activity, selection rules for IR and Raman transition.

UNIT II: **Advanced Organometallic Chemistry**

Stereochemical non rigidity and fluxional behavior of organometallic compounds with typical examples, reactions in fluxional organometallic compounds, catalysis by organometallic compounds Hydrogenation, Wilkinson Catalyst, Tolman Catalytic loop, Syntehses gas-Water gas shift reaction, Hydroformylation (Oxo process), Monsantro Acetic Acid process, Walcker process, Synthetic gasoline – Fischer Tropsch process and mobile process. Polymerization, oligomerization, and metatheses reaction of alkenes and alkynes, Zieggler Natta catalysis, Photodehydrogenation catalyst (Platinum POP).

UNIT III: **Nuclear Chemistry**

Nuclear models: Nuclear forces, liquid drop model, shell model, Fermi gas model; magic numbers, nuclear spin and nuclear isomerism. Detection and measurement of radiation. Tracer techniques. Study of chemical reactions, isotope exchange reactions, kinetic isotope effect, nuclear activation analyses, charged particle analyses. Principle of nuclear detection, gas detector, ionization chamber, proportional and G. M. detector, dead time of detectors, application of counting statistics in nuclear measurements.
Radioactive Techniques: Detection and measurement of radiation- GM ionization and proportional counters. Study of chemical reactions by tracer techniques, isotope exchange and kinetic isotope effect. Radiometric analysis: Isotope dilution analysis, age determination, neutron activation analysis (NAA) and their applications. Radiation hazards and safety measures.

CCS 515- INORGANIC CHEMISTRY SPECIALIZATION II (Credit-4)

UNIT I: **NMR, ORD/CD**

NMR: ^{1}H,^{11}B,^{13}C,^{14}N,^{17}O,^{19}F and ^{31}P-NMR: instrumentation, chemical shift and application; fluxionality, distortion and dynamic equilibria; long-range spin-spin interaction; Identification of compounds like H_3PO_3, H_3PO_2, HPF_2, P_4S_3 etc. Adduct formation reaction: AsF_3 with SO_3. Exchange reaction – exchange in H_2O, factors affecting line width, evaluation of thermodynamic parameter with NMR, determination of reaction order, rate constant etc. from NMR. NMR spectra of paramagnetic ions. Contact shifts. Factors contributing to the magnitude of chemical shift. Applications involving the magnitude of coupling constant – J_{13C-H}, J_{Pt-P}, J_{P-F} etc. NMR spectra of $B_3H_8^-$, $HP_2O_5^{3-}$, TiF_4.2B (B as donor molecule); consequences of nucleii with quadrupole moment in NMR. Double resonance technique. Introduction to pulse and FT NMR, time domain vs. frequency domain, FID, CW vs. FT NMR, rotating frame of reference, relaxation time measurements instrumentation.

CD/ORD: The symmetry origin of the optical activity of molecules, The phenomena of Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD): principle, methodology and applications, molecular dissymmetry and chiroptical properties, Cotton effect, Faraday effect in magnetic circular dichroism (MCD) and application;

UNIT II: **EPR, NQR, Mossbauer**

EPR: hyperfine splitting in various systems, factors affecting the magnitude of g-value, Anisotropy in the hyperfine coupling constants, zero-field splitting and Kramers' degeneracy, nuclear quadrupole interactions. Applications.

NQR: Basic theory, effect of magnetic field in the spectra, relationship between 'q' and molecular structure. Structural information from NQR spectra, Applications.

Mössbauer:Gamma ray emission and absorption by nuclei, Mossbauer effect — conditions, nuclear recoil, Doppler effect, instrumentation, chemical shift examples, quadrupole effect, effect of magnetic field, effect of simultaneous electric and magnetic fields, Use of Mössbauer spectra in chemical analysis, typical spectra of iron and tin compounds,

UNIT III: **I.R., Raman, Mass, PES, ESCA**

I.R., Raman: Origin, absorption of radiation by molecular vibrations in polyatomic molecules, effects giving rise to absorption bands, group vibration, limitation of the concept, FTIR, NDIR techniques. Raman Spectrometry: Theory, instrumentation, mechanism of Raman Effect, effect in solids, liquids and gases, Use of symmetry considerations to determine the number of active infra red and Raman lines, differences of IR and Raman spectra, Laser Raman spectra. Application.
EI, CI, FD, FAB-Mass, MALDI-TOF; isotropic effect, fragmentation patterns and application in structure elucidation; Photoelectron spectroscopy: Photo excitation and photo ionization, core level (XPS, ESCA) and valence level (UPS) Photoelectron spectroscopy, XPS and UPS experiment, chemical shift, detection of atoms in molecules and differention of same element in different environment from XPS, information about the nature of molecular orbital from UPS of simple diatomic molecule e. g. N_2, O_2, CO, HCl etc. ESCA: Introduction to Electron Spectroscopy for Chemical Analysis (ESCA), Application to the analysis of inorganic samples.

CCS 516- INORGANIC CHEMISTRY SPECIALIZATION III (Credit-4)

UNIT I: **Analytical techniques: Isolation, Characterization and Structure Determination**

Classification of chromatographic separation, distribution of analyte between phases, adsorption and partition chromatography, Basics of liquid chromatography, reverse and normal phase, gradient elution, solvent selection, and classes, Ion exchange and Ion chromatography, HPLC: basic concept, different detector system and simple application, GC, GL and GS chromatography: basic principle, different detectors and applications. Kinetics of solid state reaction by DTA, DSC and TGA methods, thermometric titrations.

UNIT II: **Inorganic Analyses**

Basic principle, instrumentation, special features and applications in inorganic analysis (qualitative/ quantitative as applicable) of the following techniques.

Electro analytical methods: Polarography: Ilkovic equation, half wave potential and its significance; amperometric, titrations, coulometry, cyclic voltametry, ion-selective electrode.

Flame photometric techniques: AAS, AES, and atomic fluorescence methods, ICP techniques, Fluorimetric analysis. UV-VIS-spectrophotometric methods: Photometric titration, derivative spectrophotometry, simultaneous determination of two components in a mixture.

UNIT III: **Inorganic Reaction Mechanism**

Substitution reactions in square planar, tetrahedral and octahedral geometries with special reference to d^n ion complexes: operational tests, aquation and anation, inorganic nucleophilicity scales; like Edward scale, n_{Pt} scale, Gutmann donor number, Drago E & C scale, trans effect, cis effect, reactions without metal-ligand bond breaking, water exchange rates, proton ambiguity, kinetics of chelate formation, reaction mechanisms of organometallic systems, studies on fast reactions, kinetic and activation parameters - tools to propose a plausible mechanism; stereochemical changes: types of ligand rearrangements, isomerism in 4-, 5- and 6-coordinated complexes; reactions of coordinated ligands: model choice of metal and ligand, organic synthesis with special reference to electron transfer reaction: ISM & OSM.

CCS 517- INORGANIC CHEMISTRY SPECIALIZATION IV (Credit-4)

UNIT I: **Magnetochemistry**

Different magnetic materials, experimental arrangement for determination of magnetic susceptibility: Gouy method, Faraday methiod, Vibrating sample magnetometer, SQUID, NMR method, anisotropy in magnetic susceptibility, diamagnetism in atoms and polyatomic systems, Pascal's constants , use of Pascal's constants in structure determination, two sources of paramagnetism, spin and orbital effect, spin orbit coupling, Lande interval rule, energies of J level, Curie equation, Curie law and Curie-Weiss law, First order and second order Zeeman effect, temperature independent paramagnetism, van Vleck equation and its applications, quenching of orbital contribution, magnetic properties of transition metal complexs in cubic and axially symmetric crystal field, high spin/low spin equilibrium, magnetic behavior of lanthanides and actinides, magnetic exchange interaction and magnetic materials.

UNIT II: **Solid state chemistry and X-ray crystallography**

Bonding in metal crystals: free electron theory, electrical conductivity, band theory, band gap, metal and semi-conductors –intrinsic and extrinsic semiconductors; semiconductor/metal transition, p-n junctions, superconductivity, Bardeen, Cooper and Schriefer (BCS) theory.

Dia-, para- and ferromagnetism. Defects in solids. The geometry of crystalline state; Nature and generation of X-rays, Production of monochromatic X-rays, Scattering of X-rays, Diffraction of X-rays by crystals, 1, 2 and 3 dimensional Laue equations, atomic scattering factor, structure factor, systematic absences; Determination of space groups and crystal structures. Crystal forms, lattice, primitive cell, crystal system and symmetry, non primitive lattices, crystal classes, space groups, crystals and their properties, Principle of electron, neutron and X-ray diffraction methods in determining the structure of molecules. Lattice planes, indices, Braggs condition, reciprocal lattice, Braggs law in reciprocal space.

UNIT III: **Inorganic Photochemistry**

Introduction to Inorganic Photochemistry, photophysical and photochemical processes, characteritics of the electronically excited states of inorganic compounds–ligand field states, charge transfer states, Frank-Condon, and thexi states, kinetics of photochemical process, reactivities of transition metal complexes in the ligand field and charge transfer excited states, photoelectochemistry of exicted state redox reactions, photosensitization, selective inorganic photochemistry using laser beams, Relevance of ruthenium polypyridine complexes in solar energy conversion and storage, photo splitting of water, Inorganic photochemistry in biological processes and their model studies.

CCS 518- INORGANIC CHEMISTRY SPECIALIZATION V (Credit-2)

Chemistry of Complex Equilibria

UNIT I: Different pH-potentiometric, spectrophotometric, voltammetric tools and methods (sloperatio, mole-ratio and Job's method of continuous variation) of measuring stability constants of complexes, Bjerrum half n method, stability of mixed ligand complexes and calculations; determination of composition, evaluation of thermodynamic parameters, factors influencing the stability of complexes, equilibria in biomolecular systems.

UNIT II: Characteisation of stability of mononuclear, polynuclear and mixed –ligand complexes in solution, determination of composition and stability constants of complexes by pH metric, spectrophotometric and polarographic methods. Conditional stability constants and their importance in complexometric (EDTA) titrations and solvent extraction of metal ions. Statistical and nonstatistical factors influencing stability of complexes in solution, stability and reactivity of mixed ligand complexes. Soluility Equilibria – quantitativeness of precipitation (of metal hydroxides, sulphides and chelates)

CCS 519- INORGANIC CHEMISTRY SPECIALIZATION VI (Credit-2)

UNIT I: **Synthetic Methodology for Transition and Non-transition Metal Compounds**

Ligand design and ligand synthesis: polypyridine, Schiff base, oxime, macrocycle, tripod, podand, coronand, cryptand, octopus, tailoring and appending of pendant arm, electron reservoir, ligand topology and molecular mechanics, coordination compound design and synthesis: self-assembly, structure-directed synthesis, building block, metalloligand, polymeric ensembles (chain, sheet, network), supramolecular framework, molecular machine, biomodelling, molecular/crystal engineering.

UNIT II: **Inorganic substitution reactions Mechanism**

Mechanism of substitution reactions: Solvent exchange, aquation, anation, base hydrolysis, acid catalysed aquation, pseudo-substitution. Four board classes of mechanism of substitution – 'D', 'A', 'Ia' and 'Id' Mechanism of isomerisation reaction–linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racemisation, Ray– Dutta and Bailar twist mechanisms. Mechanism of electron transfer reactions: General characteristics and classification of redox reactions, selfexchange reactions. Outer sphere and inner sphere reactions, applications of Marcus expression (simple form), redox catalysed substitution reactions.

CCS 520- INORGANIC CHEMISTRY SPECIALIZATION VII (Credit-2)

UNIT I: **Chemical Application of Group Theory**

Importance of group theory in inorganic chemistry, splitting of orbital and free ion terms in crystal fields, quantitative relationship between Oh & Td splittings, construction of energy level in infinitely strong crystal field, the effect of distortion on d-energy levels, vibronic coupling and vibronic polarization, utilization of symmetry and group theory in constructing the MO diagrams of polyatomic molecules, coordination complexes including metallocene complexes. Symmetry of normal vibration, normal mode analysis, selection rules for IR and Raman transitions.

UNIT II: **Principle of symmetry in Chemistry**

Concept of symmetry in molecules, symmetry elements and symmetry operations, combining symmetry operations. Multiplication Table by stereographic projection technique. Elements of Group Theory, Sub groups and classes of group elements. Symmetry point groups of molecules, systematic classification of molecular point groups, Application of symmetry in identifying polar and chiral molecules; Symmetry and stereo-isomerism. Unit vector transformation and interpretation of character table. Identification of symmetry label of MO in a molecule. Construction of MO on the basis of Symmetry of the molecules (H_2O, NH_3, B_2H_6, CH_4). Two dimensional space group.

CCS 521- INORGANIC CHEMISTRY SPECIALIZATION VIII (Credit-2)

UNIT I: **Catalysis**: Reduction of CO, Fischer-Tropsch synthesis and synthesis of oxygenated compound. Hydroformylation of unsaturated derivatives. Reductive carbonylation; carbonylation reactions; decarbonylation.

UNIT II: **Inorganic Polymers**: Problems and Prospects**:** Types of Inorganic Polymers, General methods of preparation, mechanical properties. Polyphosphazenes- Synthesis, properties-physical and chemical, applications including Biomedical Polysiloxanes-Preparation, analysis and testing techniques. General propertiesphysical and chemical, conformations and special configurations, interpenetrating network and co-polymers, ultra structures, applications. Polysilanes- Synthesis, properties- physical and chemical including technological. Cisplatin- Derivatives as Antiviral agents.

CCS 526- PHYSICAL CHEMISTRY SPECIALIZATION I (Credit-4)

UNIT I: **Advanced Quantum Mechanics-I**

N-dimensional vector space, matrix representation of operators, projection operators, hermitian operators. Heisenberg's uncertainty principle (operator method), Heisenberg's equation of motion, constant of motion. Virial theorem, parity and time-reversal symmetry. Angular momentum operator (in polar coordinates), commutation relation, step-up and stepdown operator. Many-electron Hamiltonian, its commutation with L^2 and L_z operators. Spin operators and Pauli spin matrices. Many electron atom and construction of wave function representing a spectroscopic state.

UNIT II: **Advanced Quantum Mechanics-II**

Perturbation Theory: (i) *Time independent formalism*: Rayleigh Schrödiger theory for nondegenerate systems; Perturbation treatment in He atom; degenerate perturbation theory, Stark and Zeeman effects. (ii) *Time dependent formalism*: Transition probability; Fermi Golden Rule; Einstein transition probabilities; spontaneous and induced emission. Derivation of spectroscopic selection rules.

UNIT III: **Statistical Mechanics-I**

Imperfect gases: Virial equation of state from grand partition function; second and third virial coefficients. Classical monatomic liquids-radial distribution function (RDF); Relating RDF with the thermodynamic properties; Integral equations; Potential of mean force; The direct correlation function.

Statistical mechanical perturbation theory of liquids: Theory and its application to derive van der Waals equation of state.

CCS 527- PHYSICAL CHEMISTRY SPECIALIZATION II (Credit-4)

UNIT I: **Group Theory-Introduction**

Symmetry Elements and Point Group: Symmetry in nature, symmetry elements and symmetry operations. Symmetry properties of atomic orbitals. Elements of group theory. Elements of group theory: groups, subgroups, classes and characters, classes of symmetry operations, symmetry point groups; representation of groups by matrices. Representation of symmetry operator transformation of basis vector, Symmetry transformation of operators; The Great Orthogonality Theorem (without proof) and its consequences; construction and applications of character tables, representation of cyclic groups. direct product and projection operator and their applications; symmetry adapted linear combination (SALC)s.

UNIT II: **Photochemistry**

Jablonski diagram, Fluorescence and phosphorescence, Delayed fluorescence, quantum yield, Mechanism and decay kinetics of photophysical processes. Fluorescence quenching (dynamic and static), Stern - Volmer equation. Energy transfer (Forster's dipole coupling), Electron Transfer phenomenon (Marcus theory, Rehm Weller theory), Proton transfer phenomenon, complex formation phenomenon (excimer, exciplex). Interaction of electromagnetic radiation with matter, Transition probabilities, Transition moment integral and its applications. Electric and megnetic dipole moments. Selection rules. Violation of Franck Condon principle, oscillator strength. Nature of transitions (e.g., $n–\pi^*$, $\pi–\pi^*$, d–d, charge transfer) solvent effect on absorption and emission spectra, Stoke's shift. Properties of electronically excited molecules: Life–time, redox potential, dipole moment, pK values. Potential energy diagram for donor acceptor system, Polarized luminescence. Nonradiative intramolecular electronic transition; internal conversion, inter-system crossing. Crossing of potential energy surface (Franck-Condon factor). Adiabatic and non adiabatic cross over. Kasha's rule.

UNIT III: **Electrochemistry**

Ion Solvent interactions: Concept, experimental determination, application to equilibria, kinetics, universal scales of potential acidity and basicity in different solvents. Born Model & Eley-Evans model, Absolute heats of hydration (Halliwel & Nyburg Method). Solvation number and its determination. Ion-solvent-non-electrolyte interactions: Salting-in and saltingout phenomena. Structure of electrified interfaces, electrical double layers and 'zeta potential'.

Ion-Association: Bjerrum and Fuoss equation for ion-pair formation. Conductance minima, Ion- triplet, Ion-quadruplets; Walden's empirical rule and Fuoss treatment of conductance minima. Fuoss Shedlovsky's method of determination of association constant.

Ion-transport in solution: Limiting Debye Huckel-Onsager Expression. (Electrophoretic effect, Relaxation effect and time of relaxation). Transport number as a function of concentration. Wien Effect, Debye-Falkenhagen effect, Nernst Hartley Expression, Viscosity B-Coefficients.

Rate equation for electrode processes; Kinetic derivation of the Nernst equation. Overvoltage. Butler-Volmer equation, Tafel equation, exchange current density. electrolytic conductance – Kohlrausch's law and its applications. Phenomenon of corrosion- electrochemical view.

CCS 528- PHYSICAL CHEMISTRY SPECIALIZATION III (Credit-4)

UNIT I: **Group Theory-Applications**

Simple applications of symmetry and group theory: Bonding and Geometry of ABn (n = 1-6) molecules; LCAO approximation, Huckel`s theory of pi-electrons, LCAO-mo-pi-bonding, three center bonding (open and closed); Crystal field splitting of free ion terms in weak and strong crystal fields (Oh and Td), energy level diagrams and symmetries and multiplicities of energy levels, effect of lowering symmetry on the d-orbital energy levels, selection rules for electronic transitions, vibronic coupling and vibronic polarization, electronically allowed transitions (Laporte selection rule); construction of MO diagrams of polyatomic molecules including coordination complexes (Oh and Td), Symmetry of normal vibrations, normal mode analysis, selection rules for vibration and Raman spectra. Correlation diagrams, Walsh diagram & its application towards molecular geometry

UNIT II: **Solid State Chemistry**

Crystalline solid – single crystal and polycrystal (twining problem); lattice; unit cell – primitive and non-primitive unit cells Unit cell parameters and crystal systems Crystal symmetry – (i) point group elements and (ii) space group elements; 32 crystal classes, HM notations, distribution in different systems and stereographic projections. Space group – HM notation, space groups in triclinic and monoclinic systems Indexing of lattice planes; Miller indeces X-ray, Cu Kα and Mo Kα radiation; X-ray diffraction; Bragg equation; Reciprocal lattice and its relation to direct lattice; Bragg reflection in terms of reciprocal lattice – sphere of reflection and limiting sphere; relation between d_{hkl} and lattice parameters. *Crystal defects and non-stoichiometry*: Schottky and Frenkel defects, colour centres. *Electronic properties*:

Kronig-Penny model, band theory, electrical and thermal conductivity of metals, semi-conductors and insulators. *Magnetic properties*: Classification of materials into dia-, para-, ferro- and antiferromagnetic types. Magnetic susceptibility and Curie's law.

UNIT III: **Polymers**

Definition and classification of polymers, including tacticity. Polymerization reactions – initiation, propagation, termination steps; inhibition, chain transfer and co-polymerization. Kinetics and mechanisms of addition and condensation polymerization, including the effect of catalysts. Crystallinity and glass temperature. Different types of polymers – electrically conducting, fire resistant, medical prosthesis, biodegradable etc. Degradation of polymers – the possible pathways and effect on the environment. Molar mass of polymers – definitions, and the different experimental techniques of determination. Thermodynamics of polymer solution. Polymer conformations.

CCS 529- PHYSICAL CHEMISTRY SPECIALIZATION IV (Credit-4)

UNIT I: **Advanced Quantum Mechanics-III**

Theoretical Treatments for Many-electron systems: (a) *Variation Method*: Variation theorem; application to ground states of different systems; extension to excited states; linear variation; (b) *Many-electron-atoms*: Many electron wave function including spin eigen functions of S^2, S_z, L^2, L_z operators, Hartree self consistent field (SCF) Method, Hatree-Fock SCF Method, Multi configuration SCF Method, Configuration Interaction (CI) Method and Density Functional Theory (DFT). (c) *Molecular Systems*: (i) Forces in molecules: Virial theorem, Hellman-Feynman theorem applications.(ii) Hückel's theory with application to simple molecular systems. The 'independent particle model' (IPM) and its limitations.

UNIT II: **Statistical Mechanics-II**

Non-equilibrium Statistical Mechanics: Random processes; Time-correlation functions; Brownian motion; Langevin equation for random motion; Random walk in one dimension; Time dependence of fluctuation; Fluctuation-dissipation theorem; Fokker- Planck equation.

UNIT III: **Non-Equilibrium Thermodynamics and Quantum Statistics**

Microscopic reversibility, Entropy production in irreversible processes. Different types of forces and fluxes, coupling of irreversible processes, phenomenological eqns. Onsager's law, Stationary states, Principle of minimum entropy production; membrane permeability, ionic conductance. Diffusion and sedimentation potentials, electrokinetic phenomena.

Thermoelectric and Thermochemical effects; Membrane transport involving biochemical reaction. Active transport.

Quantum Statistics: Liouville theorem and its consequences, its quantum version. Fermi-Dirac and Bose-Einstein distribution; their Classical limits; Application of the quantum statistics for deriving thermodynamic properties of ideal BE and FD systems (Specific heat of electron, black-body radiation, Bose Einstein condensation); density matrix.

CCS 530- PHYSICAL CHEMISTRY SPECIALIZATION V (Credit-2)

Principles & Basic Instrumentation of NMR/ESR/NQR/Mossbauer Spectra

UNIT I: *Nuclear Magnetic Resonance (NMR) Spectroscopy*: Basic instrumentation, nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift, and its measurements, factors influencing chemical sift, deshielding, spin-spin interactions, factors influencing coupling constant `J`. Classification of molecules: (ABX, AMX, ABC, A_2B_2, etc. types), spin decoupling. FT NMR (qualitative idea) and its advantages, Applications of NMR in medical diagnosis.

UNIT II: *Electron Spin Resonance (ESR) Spectroscopy*: Basic principles, zero field splitting, and Kramer`s degeneracy, factors affecting the `g` value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship.

UNIT IIII: *Nuclear Quadruple Resonance (NQR) Spectroscopy*: Qudrupole nuclei, qudrupole moments, electric field gradient, coupling constant, splitting and simple applications.

UNIT IV: *Mössbauer (MB) Spectroscopy*: Basic principle, instrumentation, spectral parameters and spectrum display, center shift, qudrupole and magnetic interactions.

CCS 531- PHYSICAL CHEMISTRY SPECIALIZATION VI (Credit-2)

Applications of NMR/ESR/Mossbauer Spectra

UNIT I: *NMR phenomenon*, spin ½ nuclei, (^{1}H, ^{13}C, ^{31}P and ^{19}F), ^{1}H NMR, Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift d, inductive and anisotropic effects on d, chemical structure correlations of d, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant J, first order patterns. Multinuclear NMR of B, Al, Si, F and P nuclei; structure and dynamics of representative inorganic molecules, deriving activation and thermodynamic parameters;

UNIT II: Introduction to 2D NMR: NOESY, COSY, HETCOR, HOMCOR, INADEQUATE, INDOR, INEPT for simple compounds and problems.

UNIT III: *ESR*: hyperfine splitting in various systems, factors affecting the magnitude of g-value, Anisotropy in the hyperfine coupling constants, zero-field splitting and Kramers' degeneracy, nuclear quadrupole interactions, Application.

UNIT IV: *Mössbauer*: Gamma ray emission and absorption by nuclei, Mössbauer effect, Isomer shift, quadrupole splitting, Application to the elucidation of structure and bonding of Fe^{III} and Fe^{II}, Sn^{IV} and Sn^{II} compounds, detection of oxidation states and inequivalent MB atoms.

CCS 532- PHYSICAL CHEMISTRY SPECIALIZATION VII (Credit-2)

Advance Molecular Spectroscopy-I

UNIT I: UV-VIS Spectroscopy: Various electronic transitions (185-800 nm), effect of solvent, Lambert-Beer law; uv-bands of saturated and unsaturated carbonyl compounds, dienes, - conjugated polyenes, Fieser-Woodward rules; uv- spectra of aromatic and heterocyclic compounds; steric effects in biphenyls.

UNIT II: IR Spectroscopy: Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic and heterocyclic compounds, ethers, phenols and amines, carbonyl compounds (aldehydes, ketones, esters, carboxylic acids, amides, anhydrides, lactones, lactams, and conjugated carbonyl compounds). Effects of solvent, hydrogen bonding on vibrational frequencies, overtones, combination bands and Fermi resonance, FT IR. Application to the elucidation of structure.

CCS 533- PHYSICAL CHEMISTRY SPECIALIZATION VIII (Credit-2)

Advance Molecular Spectroscopy-II

UNIT I: *Mass spectrometry*: Principles, basic instrumentation. Ion production – EI, CI, FI, FD, FAB and MALDI techniques. Mass-spectral fragments of organic compounds, interpretation of spectra. Application.

UNIT II: *Photoelectron spectroscopy*: Photo-excitation and photo-ionization. Core level and valence level photo-ionization (XPS, ESCA, UPS). Detection of atoms in molecules, chemical shift. Applications.

SPECILAIZED PRACTICALS

Faculty will design the course (s) according to his/her convenience/choice

CCS 510- ADVANCE ORGANIC CHEMISTRY LAB-I (Credit-2)

Preparation of organic compounds by typical organic reactions, purification and characterization of the product [by re-crystallization, TLC, PC, determination of Rf value as required, m.p/b.p.]. Characterization of organic compounds by spectroscopic means.

CCS 511- ADVANCE ORGANIC CHEMISTRY LAB-II (Credit-2)

Multistep Organic Preparation. Extraction and Purification of Natural Products and Biomolecules.

CCS 522- ADVANCE INORGANIC CHEMISTRY LAB-I (Credit-2)

Synthesis and characterization of Inorganic Compound; Preparation of transition metal complexes and their characterization.

CCS 523- ADVANCE INORGANIC CHEMISTRY LAB-II (Credit-2)

Synthesis and characterization of Inorganic Compound.

CCS 534- ADVANCE PHYSICAL CHEMISTRY LAB-I (Credit-2)

Advance physicochemical experiments.

CCS 535- ADVANCE PHYSICAL CHEMISTRY LAB-II (Credit-2)

Advance physicochemical experiments.

Syllabi for other courses will be developed later on as per requirement.

Inorganic Chemistry Books

1. Advanced Inorganic Chemistry- F. A. Cotton & G. Wilkinson, John Wiley

2. Inorganic Chemistry- J.E. Huheey, E.A. Keiter & R. L. Keiter, Harper & Row

3. Chemistry of Elements- N. N. Greenwood & A. Earnshaw

4. Concept and Models of Inorganic Chemistry-Douglass, McDaniel & Alexander

5. Coordination Chemistry- S. F. A. Kettle

6. Theoretical Approach to Inorganic Chemistry-A. F. Willams

7. Inorganic Chemistry-D. F. Shriver, P. W. Atkins & C. H. Langford

8. Chemical Applications of Group theory- F. A. Cotton

9. Molecular Symmetry & Group Theory- R. L. Carter

10. Introduction to Ligand Fields- B. N. Figgis

11. Introduction to Ligand Field Theory- C. J. Ballahausen

12. Valence- C. A. Coulson

13. Chemical Crystallography-L. W. Bunn

14. Solid State Chemistry- C. N. R. Rao

15. Ionic Crystal Lattice & Nonstoichiometry-N. N. Greenwood

16. Inorganic Reaction Mechanism- M. L. Tobe

17. Mechanism of Inorganic Reactions- Katakis & Gordon

18. Kinetics and Mechanism of Reactions of Trans. Metal Complexes- R. G. Wilkins

19. Determination and use of Stability Constants- A. E. Martell & R. J. Motekaitis

20. An Introduction to Bioinorganic Chemistry-D. R. Williams

21. Inorganic Chemistry of Biological Processes-M. N. Hughes

22. Bioinorganic Chemistry-E. I. Ochiai

23. Bioinorganic Chemistry- R. W. Hay

24. Elements of Bioinorganic Chemistry- G. N. Mukherjee & A. Das

25. Organometallic Chemistry of Transition Metals-R.H. Cabtree

26. Organometallic Chemistry- R. C. Mehrotra & A. Singh

27. Nuclear and Radio Chemistry-Friedlander, Kennedy & Miller

28. Radioactiviry Applied to Chemistry- A. C. Wahl & N. A. Bonner

29. Magnetochemistry- Selwood

30. Intriduction to Magnetochemistry- Earnshaw

31. Environmental Analysis- S. M. Khopkar

32. Physical Methods in Inorganic Chemistry-R. S. Drago

33. Instrumental Methods in Chemical Analysis- Willard, Meritt and Dean

34. Instrumental Methods in Chemical Analysis- G. W. Ewing

35. Vogel`s Text Book of Quantitative Chemical Analysis G. H. Jeffery, J. Bassett, J. Mendham & R. C. Denny

36. Advanced Experiments in Inorganic Chemistry-G. N. Mukherjee (U. N. Dhur)

37. Macro and Semi-micro Qualitative Inorganic Analysis- A. I. Vogel

38. Semi-Micro Qualitative Inorganic Analysis- G. N. Mukherjee (C.U.Press)

39. Quantitative Chemical Analysis- Kolthoff, Sandel, Meehan & Bruckenstein

40. Synthesis and Characterizations of inorganic Compounds-W. L. Jolly

41. Group Theory – Bishop (D.M.)

42. Electron Transfer reaction: ISM & OSM – Purcell & Kotz

Organic Chemistry Books

1. Organic Chemistry- I. L. Finar, Vols. 1 & 2, ELBS

2. .Adv. Organic Chemistry: Reaction, Mechanism- Jerry March

3. Adv. Organic Chemistry-F. A. Carey & R. J. Sundberg

4. Organic Chemistry (3rd. edn) -Hendrikson, Cram, Hammond

5. Organic Chemistry- Clayden, Greeves, Warren & Wolthers

6. Organic Chemistry- R. T. Morrison & R. N. Boyd

7. Organic Reaction Mechanics- A. Gallego, M. Gomer & M. A. Sierra

8. A Guide Book to Mechanism of Organic Reactions-Peter Sykes

9. Reaction Mechanism in Organic Chemistry- S. M. Mukherjee & S. P. Singh

10. Structure and Mechanism in Organic Chemistry- C. K. Ingold

11. Physical Organic Chemistry-J. Hiine

12. Physical Organic Chemistry-N. S. Isaacs

13. Orbital Symmetry and Organic Reactions-T. L. Gilchrist & R. C. Storr

14. Some Modern Methods in Organic Synthesis-W. Carruthers

15. Principles of Organic Synthesis-Norman, Coxon & Blakie

16. Current Trends in Organic Synthesis-C.Scolastico & F. Nicotra

17. Frontier Orbitals and Organic Chemcal Reactions-I. Fleming

18. Pericyclic Reactions- Gill & Willis

19. Pericyclic Reactions- S. M. Mukherjee

20. Stereochemistry-E. Eliel & S. H. Wilen

21. Stereochemistry- D. Nasipuri

21a. Stereochemistry of Organic Compounds- P. Kalsi

22. NMR in Chemistry-A Multinuclear approach—W. Kemp

23. Application of N. M. R. Spectroscopy in Organic ChemistryL- L. M. Jackman M.

24. Interpretation of ^{13}C –NMR Spectra- F. W. Werli & T. W. Wirthlin

25. Mass Spectrometry-Organic Applications-K. Biieman

26. Free Radicals in Organic Chemisrey—Fossey, Lepost & Sorbs

27. Elements of Organic Photochemistry-D. O. Cowan & K. L.Drisco

28. Application of Organotransition Metal in Organic Synthesis-S.G. Davies

29. Comprehensive Heterocyclic Chemistry- A. R. Katritzky, & C. W. Rees (eds)

30. Heterocyclic Chemistry-J. A. Joule &K. Mills

31. Natural Product-A. Pelter

32. Natural Products: Chemistry & Biological Significance Mann, Davidson, Hobbs, Banthrope, Harbome & Longman

33. An Introduction to Medicinal Chemistry-(3rd.edn) G. L. Patrick

34. Fundamentals of Medicinal Chemistry-G. Thomas

35. Supramolecular Chemistry: Concepts & Perspective- J. M. Lehn

36. Experimental Organic Chemistry: Principles & Practice-L. M. Harwood & C. J. Roodey

37. Experiments and Techniques in organic Chemistry-Pasto, Johnson & Miller

38. Spectrometric Identification of Organic Compounds-(6th. edn)-Silverstein & Webster

39. An Introduction to Experimental Organic Chemistry- Robert, Gilbert, Rodewaid & Wingrove

40. Systematic Qualitative Organic Analysis-H. Middleton

41. Hand Book of Organic Analysis- H. T. Clarke 42. Text Book of Practical Organic Chemistry-A.I. Vogel

42. Aromaticity and Aromatic Character – G.M. Badger

Physical Chemistry Books

1. Physical Chemistry: A Molecular Approach-D. A. McQuarrie & J. D. Simon

2. Physical Chemistry- R. S. Berry, S. A. Rice & J. Ross

3. Introduction to Quantum mechanics- L. Pauling & E. B. Wilson

4. Quantum Mechanics J. L. Powel & B. Crasemann

5. Elementary Quantum Chemistry-F. L. Pilar

6. Quantum Chemistry- I. N. Levine

7. Chemical Kinetics-K. J. Laidler

8. Fundamentals of Chemical Kinetics-S. W. Benson

9. Theoretical Chemistry- S. Glasstone

10. The Principles of Chemical Equilibrium-K. Denbigh

11. The Physical Chemistry of Surfaces- N. K. Adams

12. Physical Chemistry of Surfaces- A. W. Adamson

13. Introduction to Molecular Spectroscopy-G. M. Barrow

14. Fundamentals of Molecular Spectroscopy- C.W. Banwell

15. Introduction to Quantum Mechanics- D. J. Griffith

16. Group Theory and Chemistry—D. M. Bishop

17. Thermodynamics and an Introduction to Thermostatistics- H. B. Callen

18. Coulson`s Valence- R. McWeeny

19. Modern Electrochemistry-J.O`M. Bockris & A. K. N. Reddy

20. Principles of Physical Biochemistry- K. E. van Holde, C. Johnson & P. S. Ho

21. Polymer chemistry-P. J. Flory

22. Microwave Spectroscopy-C. H. Townes & A. L. Schawlow

23. Symmetry and Spectroscopy- D. C. Harris & M. d. Bertolucci

24. Solid State Physics- A. J. Dekker

25. Introduction to Solid State Physics- C. Kittel

26. Chemical Kinetics and Dynamics- J. I. Seinfeld, J. S. Francesco & W. L. Hase

27. Text Book of Physical Chemistry- S. Glasstone

28. Statistical Mechanics- D. A. Mcquarrie

29. Statistical Mechanics-B. B. Laud

30. Statistical Mechanics- K. Huang

31. Practical Physical Chemistry- A. M. James & F. F. Prichard

32. Findlay's Practical Physical Chemistry- B. P. Levit

33. Experimental Physical Chemistry- Shoemaker & Garland

34. Introduction to Magnetic Resonance-A. Carrington & A. D. McLachlan

35. NMR, NQR, EPR and Mossbauer Spectro. in Inorganic Chemistry- R. V. Parish

36. Macromolecules:Structure and Function- F. Wold, Prentice-Hall

37. Principles of Biochemistry- A.L. Lehninger

38. Programming with FORTRAN - S. Lepschutz & A. Poe (Schaum Series)

39. Computer Programming in FORTRAN 77- V. Rajaraman

40. Computational Chemistry- A. C. Norris, John Wiley

41. Computational Chemistry- A. Konar

42. Computers in Chemistry – K. V. Raman, TMH

43. Electricity and Magnetism (Vol I) – J.H. Fewkes & J. Yarwood, OUP

44. Atomic Physics (Vol II) – J. Yarwood , OUP 45. Biochemistry – Voet and Voet

45. Kinetic and Mehanism – Frost &

46. Statistical Mechanics – T.H. Hill

Computer applications in chemistry

Suggested Readings

1. Rajaraman V., Computer Progoramming in FORTRAN 90 and 95, 4th edition, Pubs:Prentice Hall, India (2004).

2. Scheid F., Numerical Analysis: Schaum's Series, Pubs: McGraw Hill, Singapore (1988)

Central University of Himachal Pradesh

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Tel: 01892-229330, 237285, Fax: 01892-229331,
Website: www.cuhimachal.ac.in

Course Code: CCS 402

Course Name: INORGANIC CHEMISTRY I

Credits Equivalent: 4 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To understand the significant aspects of Chemical bonding such as Valence band theory, Molecular orbital theory, resonance and hybridization.
2. To be able to use crystal field theory for determining Crystal field stabilization energy, lattice energy and hydration energy.
3. To be able to describe the concept of spin and orbital moments, stereochemistry of coordination compounds.
4. To be able to describe the complex chemistry, electronic configuration and magnetic properties of d and f block elements.

Course Outcomes:

The students will be able to

1. Understand the concept of valence band theory, Molecular orbital theory, hybridisation and resonance.
2. Find out the Crystal field stabilization energy, lattice energy and hydration energy.
3. Explain the spin and orbital momentum as well as stereochemistry of coordination compounds.
4. Explain the complex chemistry, electronic configuration, magnetic properties as well as factor responsible for different properties of d and f block elements.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%

- Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
- Class Attendance: 10%

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Course Code: CCS 408

Course Name: INORGANIC CHEMISTRY II

Credits Equivalent: 4 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To be able to classify organometallic compounds of transition metals on the basis of 18 electron rule and their exceptions.
2. To be able to differentiate between isolobal and isoelectronic complexes.
3. To be able to understand oxidative addition, reductive elimination reaction, insertion reactions and elimination as well as electrophilic and nucleophilic reactions;
4. To be able to identify closo, nido and arachno borane structures as well as metal carbonyls.
5. To understand the aspects of Bio-inorganic chemistry such as electron transport proteins, Fe-S proteins, ferredoxin, rubredoxin, respiratory electron transport chains as well as the harmful effects of diseases.

Course Outcomes:

The students will be able to

1. Apply 18 electron rule in order to check the stability of the complexes.
2. Understand various reactions and their mechanisms.
3. Define the structures of different boranes and carboranes.
4. Understand the functions of electron transport proteins, Fe-S proteins, ferredoxin, rubredoxin, respiratory electron transport chains.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

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Course Code: CCS 515

Course Name: INORGANIC CHEMISTRY SPECIALIZATION -II

Credits Equivalent: 2 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To understand the aspects of NMR spectroscopy such as Nuclear overhausser effect, Double resonance, Chemical exchange, Lanthanide shift reagents and NMR spectra of paramagnetic ions.
2. To understand the concepts of Nuclear Quadrupole Resonance, Nuclear electric quadrupole moment, Electric field gradient, Energy levels and NQR frequencies and Effect of magnetic field on spectra.
3. To understand the concept of Mössbauer Spectroscopy and application of MB spectroscopy in structural determination.
4. To understand the concept of Electron Spin Resonance Spectroscopy such as Hyperfine coupling in methyl, benzene and Naphthalene radicals, Factors affecting the magnitude of g-values. Zero field splitting and Kramer's Degeneracy.
5. To understand the concept of Infrared Spectroscopy as well as Raman spectroscopy.

Course Outcomes:

The students will be able to

1. Explain different aspects and processes of NMR spectroscopy.
2. Understand the concepts of Nuclear Quadrupole Resonance, Nuclear electric quadrupole moment, Electric field gradient, Energy levels and NQR frequencies and Effect of magnetic field on spectra.
3. Explain the structure on the basis of Mössbauer Spectroscopy.
4. Explain the concept of hyperfine splitting and structure on the basis of ESR spectroscopy.
5. Explain the different theories of IR absorption as well different scattering phenomenon in Raman spectroscopy.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%

2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

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Course Code: CCS 540

Course Name: - ADVANCED STEREOCHEMISTRY

Credits Equivalent: 2 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To be able to explain Optical activity, its measurement and applications.
2. To understand different chiroptical techniques like ORD and CD.
3. To be able to apply CD and ORD spectra and their correlation with biomolecules like proteins.

Course Outcomes:

The students will be able to

1. Explain empirical rules and their correlation with optical activity of different chiral molecules.
2. Understand and interpret the data of ORD and CD spectroscopy.
3. Explain the conformations of biomolecules like proteins, nucleic acids etc with help of ORD and CD spectroscopy. .

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

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Course Code: CCS 547
Course Name: BIOPHYSICAL CHEMISTRY

Credits Equivalent: 2 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To be able to explain the structure and functions of proteins and enzymes.
2. To be able to describe shapes of DNA, RNA as well as the free energy changes in biological reactions.
3. To understand the different biopolymer interactions, various binding processes and functions of cell membrane and nerve cell.

Course Outcomes:

The students will be able to

1. Explain the structure and functions of proteins and enzymes.
2. Explain the function and structure of different nucleic acids.
3. Know about the biopolymer interactions, thermodynamic aspects of biopolymer solutions and other body functions.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

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Course Code: CCS 549

Course Name: ELECTRONIC SPECTROSCOPY (ABSORPTION AND EMISSION)

Credits Equivalent: 2 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To be able to explain different principle, laws and different transitions in electronic spectroscopy.
2. To understand different processes such as deactivation – internal conversion and intersystem crossing, radiation less deactivation, fluorescence and phosphorescence.
3. To understand Quenching of fluorescence, effect of quencher, reactions of Excimers and exciplexes, Intermolecular energy transfer (FRET), Principles of LASER and its characteristic features.

Course Outcomes:

The students will be able to

1. Explain different principle, laws and different transitions in electronic spectroscopy.
2. understand different processes such as deactivation – internal conversion and intersystem crossing, radiation less deactivation, fluorescence and phosphorescence.
3. Know about Quenching of fluorescence, effect of quencher, reactions of Excimers and exciplexes, Intermolecular energy transfer (FRET), Principles of LASER and its characteristic features.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

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Course Code: CCS 559
Course Name: - Advance Analytical techniques

Credits Equivalent: 2 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:
1. To be able to explain Principle of Chromatohraphy like TLC, HPLC, and GC.
2. To understand different approaches applied in Chromatographic Techniques for Separation.
3. To be able to understand different type of detectors used in Chromatography with special emphasis on LC-MS and GC-MS.

Course Outcomes:
The students will be able to
1. Explain empirical rules and principles of Chromatographic Separation and understand different types of Chromatography and their applications.
2. Understand and interpret the data of LC-MS and GC-MS.
3. To be able to successfully design the Chromatographic separation methods and protocols for wider pool of molecules like biological and synthetic molecules.
4. **Attendance Requirements:**

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:
1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

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Course Code: CCS 566

Course Name: SPECIAL PAPER-I- ORGANIC CHEMISTRY

Credits Equivalent: 2 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To understand the aspects of mass spectroscopy and structure elucidation by mass spectroscopy.
2. To understand the concept of chemical shift, spin spin interactions and structure determination by NMR spectroscopy.
3. To understand the organometallic chemistry of transition elements.
4. To be able to use Organometallic Reagents in organic syntheses and to determine structure of Organic Compounds by IR, UV, NMR and Mass.

Course Outcomes:

The students will be able to

1. Determine the structure by Mass and NMR spectroscopy.
2. Understand the organometallic chemistry of transition elements.
3. Explain the mechanisms of organic syntheses by organometallic reagents.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

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Course Code: CCS 549
Course Name: SPECIAL PAPER-II-INORGANIC CHEMISTRY

Credits Equivalent: 2 Credits (One credit is equivalent to 10 hours of lectures / organized classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To be able to explain energy terms, orgel diagrams and splitting of terms in octahedral and tetrahedral ligand field.
2. To understand different catalyst mediated reactions and their mechanisms.
3. To be able to explain applications of nuclear chemistry as well as radioactive techniques.

Course Outcomes:

The students will be able to

1. Explain energy terms, orgel diagrams and splitting of terms in octahedral and tetrahedral ligand field.
2. Understand the reactions and mechanisms of different organocatalytic reactions.
3. Explain nuclear chemistry, radioactivity as well as radioactive techniques.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
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3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
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Course Code : CCS 409

Course Name: PHYSICAL CHEMISTRY II

Credits Equivalent: 4 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

This course enables the students,

1. To study the fundamentals and applications of classical mechanics and quantum chemistry.
2. To understand the structure of an atom and different approximation methods
3. To learn the concept of chemical kinetics and their reaction dynamics applications.
4.To Apply the molecular phenomena and spectroscopic properties of a molecules.

Course Outcomes:

On the completion of this course, Students should have to

1.Differences between classical and quantum mechanics. The limitations of classical mechanics.
2. Describe about the connection of quantum mechanical operators to observables. probabilities, amplitudes, averages, expectation values, and observables.
3. Discuss the molecular phenomena can be related to spectroscopic properties of a molecules.
4. Differentiate between common approximation methods and standard chemical frameworks (Born-Oppenheimer approximation, molecular orbitals, for example)
5. Describe about the connection of chemical kinetics and reaction dynamics.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

Course Code : CCS 403

Course Name: PHYSICAL CHEMISTRY I

Credits Equivalent: 4 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

This course enables the students

1.To learn knowledge about Thermodynamics.

2.To understand about Surface chemistry and dielectric behaviour of molecules.

3. To understand the basic concept molecular spectroscopy, structure and their properties.

Course Outcomes:

On completion of this course, students to have

1.Recognize the basic concepts of Thermodynamics.

2.Understand the valuable concepts in Surface chemistry and dielectric behaviour.

3.Discuss the basic knowledge about molecular spectroscopy and structure.

4. Predict the structure of unknown molecules by using the spectral data and to identify the structure of the molecules.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

Course Code : CCS 406

Course Name: PHYSICAL CHEMISTRY LAB I

Credits Equivalent: 2 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

This course enables the students should have

1.To get knowledge about the heat of solution, determination of molecular weight and distribution coefficient

2. To apply the basic concepts of conductometric titrations to determine the ionic strength.

3. To understand the various laws in electrochemistry.

4. To apply the conductometric method for the solutions and measure its conductivity

5. To give practice to handle the conductivity meter, spectrophotometer.

6. To evaluate distribution co-efficient influence the solubility of various systems.

Course Outcomes:

On the completion of this course, students to

1. Recognize about the heat of solution, determination of molecular weight and distribution coefficient
2. Relate the basic concepts of conductometric titrations to determine the ionic strength.
3. Understand the various laws in electrochemistry.
4. Classify the conductometric method for the solutions and measure its conductivity
5. Practice to handle the conductivity meter, spectrophotometer.
6. Criticize the distribution co-efficient influence the solubility of various systems.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

Course Code : CCS 530

Course Name: PHYSICAL CHEMISTRY SPECIALIZATION

Credits Equivalent: 2 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

This course enables the students

1. To learn knowledge about Nuclear Quadruple Resonance (NQR) spectroscopy.
2. To understand about Electron Spin Resonance (ESR) spectroscopy.
3. To understand the basic concept of NMR spectroscopy
4. To apply the different aspects of NMR spectroscopy to predict the structure of compounds.
5. To analyze about the mass spectroscopy and Mossbauer spectroscopy.

Course Outcomes:

On completion of this course, students to have

1. Recognize the basic concepts of Nuclear Quadruple Resonance (NQR) spectroscopy.
2. Understand the valuable concepts in NMR spectroscopy.
3. Discuss the basic knowledge about Electron Spin Resonance (ESR) spectroscopy.
4. Experiment the different aspects of NMR spectroscopy to predict the structure of compounds.
5. Differentiate the mass and Mossbauer spectroscopy.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

Course Code : CCS 527

Course Name: PHYSICAL CHEMISTRY SPECIALIZATION

Credits Equivalent: 4 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

This course enables the students,

1. To understand the symmetry elements and symmetry of different molecules.
2. To learn the concept of Great orthogonality theorem and character table and their applications.
3. To evaluate the concept of photochemistry to predict the spectroscopic properties of a molecules.
4. To understand the various laws in electrochemistry.

Course Outcomes:

On the completion of this course, Students should have to

1. Differences between symmetry elements and symmetry operations.
2. Describe about the connection of the Great orthogonality theorem and character table .
3. Identify the electronic transition and apply the concept of Jablonski diagram to predict the spectroscopic properties.
4. Understand the various laws in electrochemistry.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

Course Code : CCS 568

Course Name: SPECIAL PAPER-III PHYSICAL CHEMISTRY

Credits Equivalent: 2 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

This course enables the students,

1. To understand the symmetry elements and symmetry of different molecules.

2.To learn the concept of reducible and irreducible representation and their applications.

3. To evaluate the concept of group theory to predict the spectroscopic properties of a molecules.

Course Outcomes:

On the completion of this course, Students should have to

1.Differences between symmetry elements and symmetry operations.

2. Describe about the connection of the reducible and irreducible representation.

3.Identify the point groups of molecules and apply the concept of group theory to predict the spectroscopic properties.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

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Course Code: CCS 401

Course Name: Organic Chemistry I

Credits Equivalent: 4 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To impart the knowledge of different types of bonding in organic compounds.
2. To impart the knowledge of stereochemistry.
3. To impart the knowledge of asymmetric synthesis.
4. To impart knowledge about reaction mechanism.

Course Outcomes:

1. Students will be able to differentiate bonding in different compounds.
2. Students will be able to draw chiral molecules and asymmetric synthetic schemes.
3. The students will distinguish different types of reaction mechanism.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

Course Code: CCS 407

Course Name: Organic Chemistry II

Credits Equivalent: 4 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To tell the students about the basic concepts of pericyclic reactions.
2. To make them proficient to in the basic concepts of natural products.
3. To tell them about different heterocyclic compounds and their synthetic routes.

Course Outcomes:

1. Students will be able to identify the type of pericyclic reaction.
2. Students will be able to identify terpenoids and alkaloids.
3. Students will be able to know about the nitrogen, oxygen and sulfur containing heterocyclic compounds.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

4. Mid Term Examination: 25%
5. End Term Examination: 50%
6. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

Course Code: CCS 501

Course Name: CHEMISTRY GENERAL (INTERDISCIPLINARY TOPICS)

Credits Equivalent: 4 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To make the students aware about the basic techniques and concepts of nanotechnology.
2. To make them aware about supramolecular chemistry.
3. To make students aware about the different concepts in medicinal chemistry.

Course Outcomes:

1. Students will be able to distinguish the nanoparticles and tell about the nanomaterials.
2. They will be able to tell the structure activity relationship of basic drugs such as antibiotics.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

Course Code: CCS 539

Course Name: Biochemistry-II

Credits Equivalent: 4 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To make the students aware about the basic knowledge of carbohydrates, amino acids and proteins.
2. To make them aware about organometallic compounds useful in living system.
3. To make students aware about the usefulness of enzymes and Coenzymes alongwith their mode of action.

Course Outcomes:

1. Students will be able to differentiate between carbohydrate, amino acids and proteins.
2. They will be able to tell how enzymes operates in our body.
3. They will tell the role of quaternary proteins such as haemoglobin.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
   - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
   - Class Attendance: 10%

Course Code: CCS 552

Course Name: SYNTHETIC METHODOLOGY & STRATEGY

Credits Equivalent: 2 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To impart the knowledge of different reagents in organic synthesis.
2. To impart the knowledge of disconnection of organic molecules.
3. To impart the knowledge of nucleophilic substitution reactions and polymerization reaction.

Course Outcomes:

1. Students will be able to tell that which reagent can bring about the particular organic reaction.
2. Students will be able to draw synthetic schemes to synthsize organic molecules.
3. The students will tell about types of nucleophilic substitution reaction.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

1. Mid Term Examination: 25%
2. End Term Examination: 50%
3. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

Course Code: CCS 502

Course Name: Advance organic synthesis 1

Credits Equivalent: 4 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To tell the students about the basic chemistry of natural products such as terpenoids and alkaloids.
2. To make them proficient to in the knowledge of different rearrangement reactions.
3. To tell them about advanced concepts in chiral synthesis.

Course Outcomes:

1. Students will be able to identify the type of natural product.
2. Students will be able to draw main rearrangement reactions.
3. Students will be able to tell about the use of chiral auxiliary in asymmetric synthesis.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

4. Mid Term Examination: 25%
5. End Term Examination: 50%
6. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

Course Code: CCS 501

Course Name: CHEMISTRY GENERAL (INTERDISCIPLINARY TOPICS)

Credits Equivalent: 4 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To make the students aware about the basic techniques and concepts of nanotechnology.
2. To make them aware about supramolecular chemistry.
3. To make students aware about the different concepts in medicinal chemistry.

Course Outcomes:

1. Students will be able to distinguish the nanoparticles and tell about the nanomaterials.
2. They will be able to tell the structure activity relationship of basic drugs such as antibiotics.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

7. Mid Term Examination: 25%
8. End Term Examination: 50%
9. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

Course Code: CCS 503

Course Name: ORGANIC CHEMISTRY SPECIALIZATION II

Credits Equivalent: 4 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To make the students aware about charactrisation techniques such as NMR.
2. To make them aware about different chromatographic techniques.
3. To impart basic knowledge about green chemistry.

Course Outcomes:

1. Students will be able to tell the NMR spectrum of simple organic comppounds.
2. They will be able to distinguish GC and HPLC.
3. They will be able to tell how the clean synthesis can be performed in laboratory.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

10. Mid Term Examination: 25%
11. End Term Examination: 50%
12. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

Course Code: CCS 504

Course Name: ORGANIC CHEMISTRY SPECIALIZATION III

Credits Equivalent: 4 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To make the students aware about organometallic chemistry of transition metal compounds.
2. To make them aware about additional synthetic techniques.
3. To impart basic knowledge about pericyclic reactions.

Course Outcomes:

1. Students will be able to tell different types of organometallic compounds.
2. They will be able to draw synthetic schemes to complex molecules.
3. They will be able to tell distinguish different types of pericyclic reactions.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

13. Mid Term Examination: 25%
14. End Term Examination: 50%
15. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%

Course Code: CCS 505

Course Name: ORGANIC CHEMISTRY SPECIALIZATION IV

Credits Equivalent: 4 Credits (One credit is equivalent to 10 hours of lectures / organised classroom activity / contact hours; 5 hours of laboratory work / practical / field work / Tutorial / teacher-led activity and 15 hours of other workload such as independent individual/ group work; obligatory/ optional work placement; literature survey/ library work; data collection/ field work; writing of papers/ projects/dissertation/thesis; seminars, etc.)

Course Objectives:

1. To make the students aware about advanced stereochemistry.
2. To make them aware about the reagents using metals Si, S, B, Cr, Ti, Co, Rh, Ru, Pd, Cu, Ni, Fe and Ce.
3. To impart advanced knowledge of heterocyclic chemistry.

Course Outcomes:

1. Students will be able to know about different asymmetric reactions.
2. They will be able to draw R and S configurations.
3. They will be able to tell the use of reagents made up of Si, S, B, Cr, Ti, Co, Rh, Ru, Pd, Cu, Ni, Fe and Ce.
4. They can draw the synthetic schemes for complex heterocyclic molecules.

Attendance Requirements:

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75% attendance is a must failing which a student may not be permitted to appear in examination.

Evaluation Criteria:

16. Mid Term Examination: 25%
17. End Term Examination: 50%
18. Continuous Internal Assessment: 25%
    - Assignment/Library Work/Class Test/Surprise Test/Quiz: 15%
    - Class Attendance: 10%