Central University of Himachal Pradesh

Dept. of Chemistry & Chemical Sciences

School of Physical & Material Sciences

Modified Syllabus given by concerned Teachers in the Dept. of Chemistry & Chemical Sciences for Monsoon Semester 2019.

M.Sc. Chemistry Modified Syllabus.

Detail syllabi:

HUMAN MAKING COURSE

CCS 415- GREEN CHEMISTRY AND ITS APPLICATIONS (Credit -2)

UNIT I: **Introduction to Green Chemistry**

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry

UNIT II: **Principles of Green Chemistry and Designing a Chemical synthesis**

Twelve principles of Green Chemistry, solvent-free organic reactions. Green solvents– water, super critical fluids as a solvent for organic reactions, ionic liquids. Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy

UNIT III: **Examples of Green Synthesis/ Reactions and some real world cases**

Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis). Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid; microwave assisted reactions in organic solvents: Diels-Alder reaction and Decarboxylation reaction. Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction, Cannizaro reaction, Strecker synthesis, Reformatsky reaction

UNIT IV: **Future Trends in Green Chemistry**

Oxidation reagents and catalysts; Biomimetic multifunctional reagents; Green chemistry in sustainable development.

SKILL DEVELOPMENT COURSE

CCS 547- BIOPHYSICAL CHEMISTRY (Credit-2)

UNIT I: The primary, secondary, tertiary and quaternary structures of proteins and enzymes. Function of proteins and enzymes.

UNIT II: Nucleic acids: DNA, RNA, helix-coil transition, A, B and Z conformations. Free energy changes in biological reactions: ATP-ADP inter-conversion.

UNIT III: 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.

UNIT IV: 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 566- SPECIAL PAPER-I- ORGANIC CHEMISTRY (Credit-2)

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: **Organometallic Chemistry of Transitional Elements**

Preparative structural and characteristic aspects. Coupling reactions, Kumada, Heck, Sonogashira, Nigishi, Stille, Suzuki, Hyiama, Buchwald-Hartwig reactions, Tebbe's reagent, Pauson-Khand reaction. Fluctional organometallic compounds. Chemistry and use of organo-derivatives of non-transitional metals- tin, thalium, mercury, lead.

UNIT IV: **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 410- BIOPHYSICAL AND MATERIAL CHEMISTRY- (Credit-2)

UNIT-I
Cell membrane and its structure: The Cell Membrane, lipids in biological membranes, types and arrangements of proteins in membranes, lipo proteins. Bio-Energetics: Thermodynamic

Considerations: standard free energy change in bio-chemical reactions, exergonic, endergonic reactions, hydrolysis of ATP and its synthesis from ADP.

UNIT-II

Techniques for study of biomolecular structure and function- optical techniques: CD, ORD: Cotton effect, Faraday Effect, Fluorescence anisotropy for bimolecular 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 559- ADVANCE ANALYTICAL TECHNIQUES (Credit-2)

UNIT (I): Introduction to Chromatography

Basic principle of Analytical techniques. Different types of Chromatography techniques and their applications. Thin layer Chromatography – Basic principle, methodology, application.

UNIT (II): High Performance Liquid Chromatography

Basic Principle, Methodology, Application. Discussion with examples based on published research papers.

UNIT (III): Gas Chromatography

Basic Principle, Methodology, Application. Discussion with examples based on published research papers.

UNIT (IV): Liquid and Gas Chromatography - Mass spectrometry

Basic Principle, Methodology, Application. Discussion with examples based on published research papers.

CCS 538- BIOCHEMISTRY-I (Credit-2)

UNIT I: Proteins

- Amino acid : Classification and Structure
- Levels of Protein Structure
- Biologically important peptides

UNIT II: Nucleic acids and Nucleotides

- Structure of Nucleotides
- Structure and types of DNA
- Structure and types of RNA

UNIT III: Enzymes

- Classification
- Nomenclature
- Enzyme inhibition

UNIT IV: Vitamins

- Classification
- Individual vitamins
    - Chemistry
    - Biochemical functions
    - Dietary Sources
    - Deficiency symptoms

B.SC. CHEMISTRY COURSE (For Physics Honrs Students)

CCS101- CHEMISTRY I (For B. Sc. Physics) (Credit: 4)

Course Contents:

Unit I: Review of thermodynamics and the Laws of Thermodynamics. Important principles and definitions of thermochemistry. Concept of standard state and standard enthalpies of formations, integral and differential enthalpies of solution and dilution. Calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data. Variation of enthalpy of a reaction with temperature – Kirchhoff's equation.

Unit II: Thermodynamic derivation of the law of chemical equilibrium. Distinction between ΔG and ΔG_o, Le Chatelier's principle. Relationships between Kp, Kc and Kx for reactions involving ideal gases. Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle.

Unit III: Preparation (Case benzene): from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid. Reactions: (Case benzene): Electrophilic substitution: nitration, halogenation and sulphonation. Friedel-Craft's reaction (alkylation and acylation) (upto 4 carbons on benzene). Side chain oxidation of alkyl benzenes.

Unit IV: Alkyl Halides (Upto 5 Carbons) Types of Nucleophilic Substitution (SN1, SN2 and SNi) reactions. Preparation:from alkenes and alcohols. Reactions:hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation. Williamson's ether synthesis: Elimination vs substitution

Unit V: Aryl Halides Preparation*:* (Chloro, bromo and iodo-benzene case): from phenol, Sandmeyer & Gattermann reactions. Reactions (Chlorobenzene):Aromatic nucleophilic substitution (replacement by –OH group) and effect of nitro substituent. Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides. Benzyne Mechanism: KNH2/NH3 (or NaNH2/NH3).Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.

CCS 401- ORGANIC CHEMISTRY I [Credit -4]

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

Qualitative M.O. approach to bonding in organic molecules, Delocalized chemical bonding: conjugation, cross conjugation, resonance, hyperconjugation. HMO theory, Huckel`s approach to linear and monocyclic conjugated systems, its applications to ethylene, cyclopentadiene, butadiene, cyclobutadine. Antiaromaticty, aromaticity/aromatic character, homo aromaticity

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

Concept of aromaticity (η) in benzenoid and non benzenoid compounds. Alternate and non-alternate hydrocarbons, bonding in fullerenes, tautomerism, classification of tautomerism. crown ether complexes and cryptand complexes, catenanes and rotaxanes, inclusion compounds, cyclodextrins. 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, 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,; decalin, conformation of sugars. Effects of conformation on the reactivity of acyclic compounds and cyclohexanes. 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 reagents to saturated and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation involving enolates.

Semester: Ist Semester
Course code: CCS 402 **Credit-04**
Course Name: INORGANIC CHEMISTRY-I

UNIT-I: Aspects of Chemical Bonding

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. 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 and structural aspects of crystal field splitting (variation of ionic radii, lattice energy, hydration enthalpy and stability constants of complexes – Irving Williams order). Naphelauxetic Effect and Series.

UNIT-III: Theory of Coordination Chemistry-II

Labile and inert complexes. Spin and orbital moments, spin-orbit coupling, quenching of only formula, temperature dependence of magnetic moment, Super exchange 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, Determination of absolute configuration of enantiomers.

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

Lanthanide and Actinide Elements; Spectral and magnetic properties of compounds Occurrence and isolation in respect of Mo, W, Re, Pt. Synthesis, properties, reactions, structure and bonding as applicable in respect of Vaska`s complexes Lanthanide and actinide contractions and their consequences, separation of lanthanides and actinides and their applications

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.

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 ; Microcanonical ensemble, Canonical ensemble distribution probability partition function, its relation with different thermodynamic state functions.

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.
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.

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 568- SPECIAL PAPER-III- PHYSICAL CHEMISTRY (Credit-02)

UNIT-I

The concept of group, Symmetry elements and symmetry operations, 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.

UNIT-II

Assignment of point groups to Inorganic molecules, Some general rules for multiplications of symmetry operations, Multiplication tables for water and ammonia, Representations (matrices, matrix representations for C_{2V} and C_{3V} point groups irreducible representations), Character and character tables for C_{2V} and C_{3V} point groups.

UNIT-III

Applications of group theory to chemical bonding (hybrid orbitals for σ-bonding in different geometries and hybrid orbitals for π-bonding.

UNIT-IV

Application of Group Theory in Vibrational Spectroscopy: A brief idea about Infrared and Raman scattering spectroscopy. Vibrational modes as basis of group representations w.r.t. SO_2, $POCl_3$, $PtCl_4^{2-}$ and RuO_4, Mutual exclusion principle.

SEMSTER: 3rd Semester 2019
Course Code: CCS 411
Course Name: Statistical error, Electrochemical analyses, Environmental analyses (2 Cr.hrs)

UNIT I: Accuracy and precision of analytical procedure; Types of errors in quantitative analyses: systematic errors and random errors; Propagation of Error

UNIT II: Presentation of analytical results: descriptive statistics, Normal and Gaussian distribution and its properties, standard deviation, normal distribution of mean, confidence limits of the mean; regression and correlation

UNIT III Sampling and sample preparation: Sample plan, sample preservation, sample pretreatment, Extraction techniques used in sample preparation (Classical methods and solid phase extraction, Supercritical fluid extraction, micro-wave extraction, Pressurized Liquid extraction). Method validation (Figure of merits).

UNIT III: Atmospheric Aerosols:$PM_{2.5}$ and $PM_{1.0}$; Health implications of atmospheric aerosols; Methods of determination of $PM_{2.5}$ and $PM_{1.0}$ aerosols concentration Toxic chemical species associated with atmospheric aerosols; heavy metals, poly-nuclear aromatic hydrocarbons (PAHs) and pesticides etc. Application of electrochemical analytical (including Voltammetric) methods to determine heavy metals.

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

UNIT I: **Supramolecular Chemistry**

Introduction, Origins and Concept. Molecular recognition. Host-guest complex. Supramolecular reactivity and catalysis. Self-assembly, Liquid crystals and supramolecuar polymers, Supramolecular interactions; van der Waal interactions, dipole-dipole, pi-pi interactions. Allosterism, proton and hydride sponges, Anion recognition and anion coordination chemistry.

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

Different types of receptors with special reference of Crown ethers, cryptates and Calix[4]arene, superstructures in organometallic compounds, supramolecular devices, dendrimers. Applications 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. Bottom up and top down approaches. Synthesis of nanoparticles by chemical routes (sol-gel synthesis, micro emulsion technique, hydrothermal synthesis, polyol synthesis) and characterization techniques: TEM; SEM; AFM; XPS. Properties of nanostructured materials: Optical properties; magnetic properties; chemical properties. Microporous material, microgels, bioconjugate polymers, Nanoencapsulation.

UNIT IV: **Medicinal Chemistry**

Drugs: Introduction Drug design, Classification of drugs, brief discussion of drug targets, Drugs based on enzyme inhibition: penicillin antibiotics and sulphonamides (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 penicillin antibiotic and sulphonamides. Concept of LD_{50} and ED_{50}. Cardiovascular drugs.

CCS 540- ADVANCED STEREOCHEMISTRY- (Credit-2)

UNIT I: **Stereochemistry of polycyclic system:**

a) Dynamic Aspects**:** Cyclisation reactions, Baldwin Rule; elimination, addition and rearrangement reactions.

b) Stereospecific and stereoselective reaction, asymmetric synthesis, absolute asymmetric synthesis, Sharpless epoxidation reaction, Sharpless dihydroxylation, stereochemistry of some important reactions. (Aldol reaction, Witting reaction and Diel's Alder reaction)

c) Conformation and reactivity of fused polycyclic systems perhydrophenanthrenes, perhydroanthracene, steroids.

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.

Semester: 3rd Semester
Course code: CCS 567-SP II **Credit-02**
Course Name: INORGANIC CHEMISTRY SPECIALIZATION II

UNIT I: Group theory and its Applications in Spectroscopy

Selection rules and its relaxation, Energy Terms and Orgel diagram, splitting of terms in octahedral and tetrahedral ligand fields,

UNIT II: Advanced Organometallic Chemistry

Catalysis by organometallic compounds: Tolman Catalytic loop, Hydrogenation, Wilkinson Catalyst, Polymerization -Zieggler Natta catalysis, Phase transfer catalyst (PTC), Synthesis gas-Water gas shift reaction, Hydroformylation (Oxo process), Monsantro Acetic Acid process, Walcker process, Synthetic gasoline – Fischer Tropsch process and metatheses reaction,

UNIT III: Application of Nuclear Chemistry

Nuclear stability,Nuclear cross-sections, Nuclear reactions: types of reactions, Nuclear fission-fission product and fission yields,

Radioactive techniques: Tracer technique, (neutron activation analysis), Counting techniques such as G.M. Ionization and proportional counters.