Department of Chemistry

Module of Syllabus: 2023-24 (under CCF)

CHEMISTRY MINOR-I

Semester	Paper	Unit	Sub unit	Name of the Faculty	No. of lectures
I	CHEM-MN-1	**Module:1** Extra nuclear structure of atoms and Periodicity	1. Wave-Particle duality; de Broglie hypothesis. Heisenberg's uncertainty principle	SG	1
			2. Introducing Schrödinger equation. Hydrogen and hydrogen like systems (detailed solution not required)		2
			3. Concept of Atomic Orbital ; shapes of s, p and d orbitals . Radial and angular distribution curves. Extension to multielectronic systems		2
			4. Aufbau principle and its limitations; Pauli's exclusion principle, Hund's rules and multiplicity.		1
			5. Effective nuclear charge. Shielding and penetration; Slater's rule.		1
			6. The general idea about modern periodic table, atomic and ionic radii		1
			7. Ionization energy, electron affinity and electro negativity –definition, trends of variation in periodic table and their application in explaining and predicting the chemical behavior of elements and compounds		1
			8. Electronegativity scales Pauling's, Mulliken's and Allred-Rochow's scales). Inert pair effect.		1

		Module-II Basics of Organic Chemistry Bonding and Physical Properties: (10 Lectures)	**A. Valence Bond Theory** 1. Nomenclature of Organic Compounds 2. Concept of hybridisation, shapes and structures of molecules 3. Double bond equivalent (DBE) 4. Resonance (including hyperconjugation) and Resonance energy. 5. Electronic displacements Inductive effect, bond polarization and bond polarizability; steric effect, steric inhibition of resonance.	SG	 1 1 1 1 1
			B. MO Theory 1. Qualitative idea about molecular orbitals, bonding and antibonding interactions, idea about σ, σ*, π, π *, n – MOs; concept of HOMO, LUMO and SOMO, sketch and energy levels of π MOs of i) acyclic p orbital system (C=C, conjugated diene, triene, allyl and pentadienyl systems) 2. ii) cyclic p orbital system (neutral systems: [4], [6] annulenes; 3. charged systems:3-,4-,5-7 membered ring systems 4. Hückel's rules for aromaticity up to [8] annulene; concept of antiaromaticity; non-aromatic molecules.	SG	 1 1 1 1
			C. **Physical properties** 1. Melting point/boiling point and solubility of common organic compounds in terms of covalent & non-covalent intermolecular forcesPolarity of molecules and dipole moments	SG	1

			D. **Stereochemistry** – I: 1. Bonding geometries of carbon compounds and representation of molecules: tetrahedral nature of carbon and concept of asymmetry 2. Fischer, sawhorse, flying wedge and Newman projection formulae and their inter translations 3. Concept of chirality and symmetry: symmetry elements, molecular chirality and centre of chirality 4. Asymmetric and dissymmetric molecules; enantiomers and diastereomers; concept of stereogenicity, chiral centres and number of stereoisomers: systems involving 1/2-chiral centre(s).	SG	 1 1 1 1
		Module : III Thermodynamics -I	1. Concept of systems (open , closed and isolated) and surroundings . State of a system Intensive and extensive variables. Partial derivatives. Exact and inexact differentials. Path function and State function 2. Concept of heat and work. zeroth law of thermodynamics, Concept of thermodynamic reversibility. Concept of internal energy and 1st law of thermodynamics 3. Enthalpy and heat capacity, Relations between Cp and Cv . Isothermal and Adiabatic processes, Calculations of ΔU , ΔH , q and w involving ideal gases in different processes. 4. Enthalpy of reaction. Hess's law. Enthalpy of formation and combustion,Kirchhoff's equation.	SC	2 2 2 2
		Chemical Kinetics-I:	1. Concept of order and molecularity. Rate laws for zero, 1st order reactions and in general for any n-th order reaction 2. 2nd order reactions and in general for any n-th order reaction. 3. Determination of order of a reaction by half-life and differential methods. Rate determining	SC	1 1 2

			step and steady state approximation. Opposing, Consecutive and parallel reactions (first order steps only).Temperature dependence of rate constant and Arrhenius equation		
		Practical	1. Calibration and use of apparatus. (2) Preparation of primary standard solutions (Oxalic Acid and K2Cr2O7) **Acid-Base Titrations:** 3) Standardization of NaOH standard oxalic acid solution. (4) Estimation of Carbonate and bicarbonate present together in a mixture 5) Estimation of acetic acid in commercial Vinegar. **Oxidation-Reduction Titrimetry:** 6) Standardization of KMnO4 standard Oxalic Acid solution. 7) Estimation of Fe(II) using standardized KMnO4 solution. 8) Estimation of Fe(III) using standard K2Cr2O7 solution. 9) Estimation of Fe(II) and Fe(III) in a given mixture using standard K2Cr2O7 solution.	SG	1 1 1 1 1 1 1 1

CHEMISTRY MINOR-II

Paper	Unit	Sub unit	Name of the Faculty	No. of lectures
CHEM-MIN-II	Module : I Kinetic Theory and Gaseous state:	1. Concept of pressure and temperature from kinetic theory of gas. Nature of distribution of velocities, Maxwell's distribution of speeds in one, two and three dimensions 2. Kinetic energy distribution in one, two and three dimensions, calculations of average, root mean square and most probable values in each case; Collision of gas molecules 3. Collision diameter; Collision number and mean free path; Frequency of binary collisions (similar and different molecules) 4. Wall collision and rate of effusion Calculation of number of molecules having energy ≥ ε, Principle of equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases.	SC	1 2 1 2
	Real gas and Virial equation:	1. Deviation of gases from ideal behavior; compressibility factor; Boyle temperature; Andrew's and Amagat's plots 2. Van der Waals equation and its features; its derivation and application in explaining real gas behavior, other equations of state 3. Existence of critical state, Critical constants in terms of van der Waals constants; 4. Law of corresponding states; virial equation of state; van der Waals equation expressed in virial form and significance of second virial coefficient 5. Intermolecular forces (Debye, Keesom and London interactions; Lennard-Jones potential - elementary idea)	SC	1 1 1 2 1

	Module : II Chemical Bonding-I	i) **Ionic bond:** 1. General characteristics, types of ions, size effects, radius ratio rule and its application and limitations. Packing of ions in crystals. Born-Lande equation with derivation and importance of Kapustinskii expression for lattice energy. 2. Madelung constant, Born-Haber cycle and its application. Solvation energy. 3. Defects in solids (elementary idea). Solubility energetic of dissolution process.	SG	1 1 1
		ii) **Covalent bond:** 1. Polarizing power and polarizabilty, ionic potential, Fajan's rules, Lewis structures, formal charge 2. Valence Bond Theory, The hydrogen molecule (Heitler – London approach), directional character of covalent bonds, hybridizations, equivalent and non-equivalent hybrid orbitals 3. Bent's rules, dipole moments, VSEPR theory, shapes of molecules and ions containing lone pairs (examples from main group chemistry) and multiple bonding (σ and π bond approach).	SG	1 1 1
	Theoretical principles of inorganic qualitative analysis:	1. Basic principles involved in analysis of cations and anions and solubility products, common ion effect. Principle involved in separation of cations into groups and choice of group reagents. 2. Interfering anions (fluoride, borate, oxalate and phosphate) and need to remove them after Group II.	SG	1 1
	Module: III Stereochemistry – II	1. Chirotopicityand its relationship with stereogenicity; concept of pseudoasymmetry for ABA type systems. 2. Relative and absolute configuration: R/S descriptors; erythro/threo and meso nomenclature of compounds, E/Z descriptors for C=C, combination of R/S- and E/Z isomerisms.	SG	1 2

		3. Optical activity of chiral compounds: optical rotation, and specific rotation; racemic compounds, racemisation (through cationic, anionic intermediates); resolution of acids and bases via diastereomeric salt formation; optical purity and enantiomeric excess.		3
	General Treatment of Reaction Mechanism–I:	**A. Reactive intermediates:** 1.Carbocations (carbenium and carbonium ions), non-classical carbocations, 2. Carbanions, carbon radicals: generation and stability, structure and electrophilic / nucleophilic behaviour of reactive intermediates (elementary idea). **B. Reaction thermodynamics:** Free energy and equilibrium, enthalpy and entropy factor, calculation of enthalpy change via BDE, intermolecular & intramolecular reactions. **C. Reaction kinetics:** Rate constant and free energy of activation; free energy profiles for one-step, and two-step reactions; catalyzed reactions, principle of microscopic reversibility; Hammond's postulate. **D. Substitution reaction:** Free-radical substitution reaction: halogenation of alkanes, mechanism (with evidence) and stereochemical features; reactivity-selectivity principle in the light of Hammond's postulate.	SG	1 1 1 1 1
	MN-II Practical	Qualitative semimicro analysis of mixtures containing three radicals. (only water /acid soluble salts): Cation Radicals Na+, K+, Ca2+, Sr2+, Ba2+, Al3+, Cr3+, Fe3+, Mn2+/Mn4+, Co2+/Co3+, Ni2+, Cu2+, Zn2+, Pb2+, NH4 +, Sn2+/Sn4+ Anion Radicals F- , Cl- , Br- , I- , S2O3 2- , S2- , SO4 2- , NO3 - , NO2 - , PO4 3- , BO3 3- , CrO4 2- / Cr2O7 2 , SCN- , [Fe(CN)6] 3- , [Fe(CN)6] 4- , AsO4 3- , BrO3 - , IO_3^-	SG	10