Department of Applied Chemistry and Basic Sciences

Syllabus for PhD. Entrance Test Pharmaceutical Chemistry (M.Sc. based)

Unit I Structure, formation, reaction, stereochemistry and stability of Carbocation, Carbanions, free radicals, carbene, and nitrene. Mechanism involving free radical, nucleophile & electrophile mediated reactions. SN1, SN2 and mixed SN1 and SN2 mechanism and its stereo chemical aspects. Factor influencing neucleophilic substitution reactions, Reactivity effects of substrate structure, attacking nucleophilic group, leaving group and reaction medium, ambient nucleophile. Mechanisms involving Aromatic electrophilic reaction, Aromatic nucleophilic reactions, free radical reactions and elimination mechanism. Mechanism and stereo chemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemo selectivity, orientation and reactivity. Addition to cyclo propane ring. Geometrical isomerism & stereochemistry of olefins. Stereoisomerism of rings, stability of rings, ease of ring formation, Actual shape of six membered rings & its relation to properties & reactivity. Optical rotation, its significance, instrumentation.Optical rotatory dispersionterminology, plain curve, rotatory dispersion & circular dichroism and octane rule.

Unit II Chromatography: principles , instrumentation and application of following separation techniques Paper chromatography, Thin layer chromatography, Column chromatography, HPLC, GC, HPTLC, Electrophoresis, Ion exchange and Gel filtration chromatography. UV-Visible spectroscopy: Theory, absorption law, Colorimetric Methods, Chromophore and auxochrome concept, Solvent effect, Instrumentation and applications, Woodword's Fieser, Fieser Kuhn and Nelson rule, Spectral correlation with structures. Atomic spectrophotometry: Atomic emission & Atomic absorption spectrophotometry: principle, instrumentation, interferences and applications. Infrared spectroscopy, Interpretation of IR, spectra of simple compounds. NMR, Spectrometry: Principle, ionization techniques, instrumentation, fragmentation pattern & applications. GC-MS and LC-MS: Principle, Instrumentation and Applications.

Unit III Carbohydrate : Introduction, classification, mutarotation, constituent of glucose, ring structure of glucose, configuration of monosaccharides, structure elucidation of disaccharides- sucrose, maltose, lactose, polysaccharides- starch. Glycosides arbutin ,amygdaline. Alkaloids : General introduction, distribution in plants, classification, isolation & purification. General methods of structure determination. Structural elucidation of atropine, quinine, Nicotin, Terpenoids : General introduction, classification, isolation & purification, isoprene, structure elucidation of citral, menthol, camphor, Structures of abietic acid and β-carotene. Plant Pigments: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of cyanidin, and quercetin. Porphyrins: General Introduction of haemoglobin and chlorophyll. Chemistry of chlorophyll (without synthesis). Structure and synthesis of haem. Heterocyclic compounds: General chemical behaviour of aromatic heterocycles, classification (structural type), Heteroaromatic reactivity and tautomerism in aromatic heterocycles Strain –bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of sixmembered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interactions. Stereo-electronic effects, aromatic and related effects. Attractive interactions - hydrogen bonding and intermolecular nucleophilic, electrophilic interactions., Small Ring Heterocycles: Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes, Benzo-Fused Five-Membered Heterocycles: Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes, Six-Membered Heterocycles with One, Two or More Heteroatoms: Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridines Synthesis and reactions of

quinolizinium and benzopyrylium salts, coumarins and chromones Synthesis and reactions of diazines, triazines, tetrazines and thiazines

Unit-IV Concept of isosterism and bioiososterism and their applications in drug design, Antimetabolite approach to drug design, Analog drug design, Prodrugs and drug latentiation – Carrier-linked prodrugs – Bioprecursors – Role of functional groups in prodrug design, General pathways of drug metabolism Specific and non-specific drug action , Drug receptors, Basic concept and classification of receptors, Forces involved in drug receptors- interactions , Receptor agonism and antagonism , Stereochemical aspects of drug action – Setereoselectivity of optical isomers – Role of planarity in drug action – Stereoselectivity of conformational isomers,

Unit-V Green chemistry: History, need, and goals. Green chemistry and Sustainability. Dimensions of sustainability, Limitations/Obstacles in pursuit of the goals of Green Chemistry. Opportunities for the next generation of materials designers to create a safer future. Hazard assessment and mitigation in chemical industry , Future trends in Green Chemistry: Oxidation-reduction reagents and catalysts, Statistical data analysis: Accuracy and precision, significant figures and computations, mean and standard deviation, distribution of random errors, reliability of results, confidence interval, comparison of results, comparison of means of two samples, paired t-test, number of replicate determinations and its use, correlation and regression, linear regression, analysis of variance, rejection of data.

Unit- VI Basics of Drug Action General principles, Identification and study of targets for development of various therapeutic agents, Rational approach for drug design, Computer aided drug design, QSAR, Molecular modelling, Combinatorial Chemistry, Study of recently developed drugs and molecules in development pipeline. Concept of isosterism and bioiososterism and their applications in drug design, Antimetaboliteapproach to drug design, Analog drug design, Prodrugs and drug latentiation, Carrierlinked prodrugs, Bioprecursors, Role of functional groups in prodrug design, General pathways of drug metabolism Specific and non-specific drug action, Drug receptors, Basic concept and classification of receptors, Forces involved in drug receptors- interactions , Receptor agonism and antagonism , Stereochemical aspects of drug action Setereoselectivity of optical isomers,Role of planarity in drug action,Stereoselectivity of conformational isomers

Chemistry (M.Sc. based)

Unit I Structure and bonding in homo- and heteronuclear molecules, including shapes of molecules (VSEPR Theory).Main group elements and their compounds: Allotropy, synthesis, structure and bonding, industrial importance of the compounds.Transition elements and coordination compounds: structure, bonding theories, spectral and magnetic properties, reaction mechanisms.Inner transition elements: spectral and magnetic properties, redox chemistry, analytical applications. Organometallic compounds: synthesis, bonding and structure, and reactivity. Organometallics in homogeneous catalysis. Cages and metal clusters. Bioinorganic chemistry: photosystems, porphyrins, metalloenzymes, oxygen transport, electron- transfer reactions; nitrogen fixation, metal complexes in medicine. Solid state: Crystal structures; Bragg's law and applications; band structure of solids

Unit II Basic principles of quantum mechanics: Postulates; operator algebra; exactly- solvable systems: particle-in-a-box, harmonic oscillator and the hydrogen atom, including shapes of atomic orbitals; orbital and spin angular momenta; tunneling.Chemical applications of group theory; symmetry elements; point groups; character tables; selection rules.Chemical thermodynamics: Laws, state and path functions and their applications; thermodynamic description of various types of processes; Maxwell's relations; spontaneity and equilibria; temperature and pressure dependence of thermodynamic quantities; Le Chatelier principle; elementary description of phase transitions; phase equilibria and phase rule; thermodynamics of ideal and non-ideal gases, and solutions.Chemical kinetics: Empirical rate laws and temperature dependence; complex reactions; steady state approximation; determination of reaction mechanisms; collision and transition state theories of rate constants; unimolecular reactions; enzyme kinetics; salt effects; homogeneous catalysis; photochemical reactions.

Unit III Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction. Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.Common named reactions and rearrangements – applications in organic synthesis.Pericyclic reactions – electrocyclisation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Principles and applications of photochemical reactions in organic chemistry.

Unit IV Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S), Chemistry of natural products: Carbohydrates, proteins and peptides, fatty acids, nucleic acids, terpenes, steroids and alkaloids.Polymer chemistry: Molar masses; kinetics of polymerization

Unit V Characterisation of inorganic compounds by IR, Raman, NMR, EPR, Mössbauer, UV-vis, NQR, MS, electron spectroscopy and microscopic techniques. Nuclear chemistry: nuclear reactions, fission and fusion, radio-analytical techniques and activation analysis. Structure determination of organic compounds by IR, UV-VIS, 1H & 13C NMR and Mass spectroscopic techniques

Dr. Neetu Pandey
Incharge Applied Chemistry and Basic Sciences