BRANCH VB

M.Sc.
PHARMACEUTICAL
CHEMISTRY

FOREWORD

I feel highly privileged in presenting the revised curricula and syllabi of Branch VB M.Sc. Pharmaceutical Chemistry for favour of approval by the Faculty and Academic Council of the University.

As per Mahatma Gandhi University PG Programme Regulations for Credit Semester System 2011(MGU-CSS-PG) it has been decided to introduce the Credit Semester System for all the PG courses which are being offered by the affiliated colleges/institutions of the University with effect from the academic year 2012-2013 admission onwards. The PG Board of Studies in Chemistry was entrusted with the duty of preparing the revised curricula and syllabi for all the five M.Sc. Programmes in Chemistry currently approved by the University and offered in the affiliated colleges.

The BOS prepared draft proposals of revised curricula and syllabi for all the M.Sc. courses in Chemistry in conformity with the broad guidelines issued by the University to suit the Credit Semester System. The draft curricula and syllabi for all the five M.Sc. Programmes were discussed in a very effective manner with active participation of Resource Persons and Teacher Representatives from all the colleges in a three-day workshop. The workshop was a grand success and the BOS could incorporate many of the suggestions while finalizing the proposal of the Restructured Curricula and Syllabi.

The BOS feel that appreciable updating could be done in keeping with the current developments and trends in chemistry education. The task of preparing the Curricula and Syllabi and bringing it out in the present form for all the five M.Sc. courses was not a simple task but it was possible with dedicated efforts and wholehearted support and involvement of all the members of the BOS. I would like to express my sincere thanks to all my fellow members of the BOS for all their whole hearted time-bound help, cooperation and encouragement. It has been a pleasure for me to work with them. I am also thankful to all Resource Persons and Teacher Representatives of the colleges for their active participation and useful suggestions during the three-day workshop.

Prof. (Dr.) P. K. Radhakrishnan
Chairman, PG Board of Studies in Chemistry

PG Board of Studies in Chemistry

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	S.I.No.	Course	Hours/ Week	Total Hours	Credit
Semester 1	PH1C01	Organometallics and Nuclear Chemistry	4	72	4
	PH1C02	Structural and Molecular Organic Chemistry	4	72	4
	PH1C03	Quantum chemistry and Group Theory	4	72	4
	PH1C04	Classical and Statistical Thermodynamics	3	54	3
	PH2P01	Inorganic Chemistry Practical	3	54	Evaluation at the end of second semester
	PH2P02	Organic Chemistry Practical	3	54	
	PH2P03	Physical Chemistry Practical	4	72	
		Total	**25**	**450**	**15**
Semester 2	PH2C05	Coordination Chemistry	4	72	4
	PH2C06	Organic Reaction Mechanisms	4	72	4
	PH2C07	Chemical Bonding and Computational Chemistry	4	72	4
	PH2C08	Molecular Spectroscopy	3	54	3
	PH2P01	Inorganic Chemistry Practical	3	54	3
	PH2P02	Organic Chemistry Practical	3	54	3
	PH2P03	Physical Chemistry Practical	4	72	3
		Total	**25**	**450**	**24**
Semester 3	PH3C09	Synthetic and Bioorganic Chemistry	4	72	4
	PH3C10	Physical Chemistry	4	72	4
	PH3C11	Drug Design and Pharmacology	4	72	4
	PH3C12	Spectroscopic Methods in Chemistry	3	54	3
	PH4P04	Pharmaceutical Analysis Practical	3	54	Evaluation at the end of fourth semester
	PH4P05	Drug Synthesis and Dispensing Practical	3	54	
	PH4P06	Biochemistry and Bacteriology Practical	4	72	
		Total	**25**	**450**	**15**
Semester 4		Elective 1	5	90	4
		Elective 2	5	90	4
		Elective 3	5	90	4
	PH4P04	Pharmaceutical Analysis Practical	3	54	3
	PH4P05	Drug Synthesis and Dispensing Practical	3	54	3
	PH4P06	Biochemistry and Bacteriology Practical	4	72	3
	PH4D01	Project			3
	PH4V01	Viva			2
		Total	**25**	**450**	**26**
Grand Total					**80**

SEMESTER 1

PH1C01 ORGANOMETALLICS AND NUCLEAR CHEMISTRY

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Organometallic Compounds- Synthesis, Structure and Bonding (18 Hours)

1.1 Organometallic compounds with linear pi donor ligands-olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding.

1.2 Complexes with cyclic pi donors-metallocenes and cyclic arene complexes-structure and bonding. Hapto nomenclature. Carbene and carbyne complexes.

1.3 Preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls with and without bridging. Carbonyl clusters-LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons.

Unit 2: Reactions of Organometallic Compounds (9 Hrs)

2.1 Substitution reactions-nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands.

2.2 Addition and elimination reactions-1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion (migration) and elimination reactions.

2.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

Unit 3: Catalysis by Organometallic Compounds (9 Hrs)

3.1 Homogeneous and heterogeneous organometallic catalysis-alkene hydrogenation using Wilkinson catalyst, Tolman catalytic loops.

3.2 Reactions of carbon monoxide and hydrogen-the water gas shift reaction, the Fischer-Tropsch reaction(synthesis of gasoline).

3.3 Hydroformylation of olefins using cobalt or rhodium catalyst.

3.4 Polymerization by organometallic initiators and templates for chain propagation-Ziegler Natta catalysts.

3.5 Carbonylation reactions-Monsanto acetic acid process, carbonylation of butadiene using $Co_2(CO)_8$ catalyst in adipic ester synthesis.

3.6 Olefin methathesis-synthesis gas based reactions, photodehydrogenation catalyst ("Platinum Pop"). Palladium catalysed oxidation of ethylene-the Wacker process.

Unit 4: Organometallic Polymers **(9 Hrs)**

4.1 Polymers with organometallic moieties as pendant groups, polymers with organometallic moieties in the main chain, based condensation polymers, condensation polymers based on ferrocene and on rigid rod polyynes, polymers prepared by ring opening polymerization, organometallic dendrimers.

Unit 5: Bioinorganic Compounds **(18 Hrs)**

5.1 Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin and crown ether complexes of Na^+ and K^+, ATP and ADP. Photosynthesis-chlorophyll a, PS I and PS II. Role of calcium in muscle contraction, blood clotting mechanism and biological calcification.

5.2 Oxygen carriers and oxygen transport proteins-haemoglobins, myoglobins and haemocyanin, haemerythrins and haemevanadins, cooperativity in haemoglobin. Iron storage and transport in biological systems-ferritin and transferrin. Redox metalloenzymes-cytochromes, peroxidases and superoxide dismutase and catalases. Nonredox metalloenzymes-CarboxypeptidaseA-structure and functions. Nitrogen Fixation-nitrogenase, vitamin B_{12} and the vitamin B_{12} coenzymes.

5.3 Metals in medicine-therapeutic applications of *cis*-platin, radio-isotopes and MRI agents. Toxic effects of metals(Cd, Hg, Cr and Pb).

Unit 6: Nuclear Chemistry **(9 Hrs)**

6.1 Fission products and fission yield. Neutron capture cross section and critical size. Nuclear fusion reactions and their applications. Chemical effects of nuclear transformations. Positron annihilation and autoradiography. Principles of counting technique such as G.M. counter, proportional, ionization and scintillation counters. Cloud chamber.

6.2 Synthesis of transuranic elements such as Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium and elements with atomic numbers 104 to 109.

6.3 Analytical applications of radioisotopes-radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, Radioanalysis, Neutron Activation Analysis, Prompt Gama Neutron Activation Analysis and Neutron Absorptiometry.

6.4 Applications of radio isotopes in industry, medicine, audiography, radiopharmacology, radiation safety precaution, nuclear waste disposal. Radiation chemistry of water and aqueous solutions.

6.5. Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.

References

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03. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.

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09. S.N. Goshal, Nuclear Physics, S. Chand and Company, 2006.

PH1C02 STRUCTURAL AND MOLECULAR ORGANIC CHEMISTRY

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Basic Concepts in Organic Chemistry (18 Hrs)

1.1 Review of basic concepts in organic chemistry: bonding, hybridisation, MO picture, inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.

1.2 The formalism of curved arrow mechanisms. Practicing of line diagram drawing.

1.3 Concept of aromaticity: delocalization of electrons - Hückel's rule, criteria for aromaticity, examples of neutral and charged aromatic systems - annulenes. NMR as a tool for aromaticity. Anti-and homo-aromatic systems - Fullerenes, Carbon nanotubes and Graphene.

1.4 Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. SN1, SNAr, SRN1 and Benzyne mechanisms.

Unit 2: Physical Organic Chemistry and Photochemistry (18 Hrs)

2.1 Energy profiles. Kinetic versus thermodynamic control of product formation, Hammond postulate, kinetic isotope effects with examples, Hammet equation, Taft equation.

2.2 Catalysis by acids and bases and nucleophiles with examples from acetal, cyanhydrin and ester formation and hydrolysis reactions –A_{AC}^2, A_{AC}^1, A_{AL}^1, B_{AC}^2 and B_{AL}^1 mechanisms, solvent effect. Linear free energy relationship. Bulk and specific solvent effects. Introduction to carbon acids - pKa of weak acids, kinetic and thermodynamic acidity. Hard and soft acids and bases - HSAB principle and its applications.

2.3 Photoreactions of carbonyl compounds: enes, dienes, dienones and arenes. Norrish reactions of acyclic ketones. Patterno-Buchi reaction. Barton, Di-π-methane and photo Fries rearrangements. Photochemistry of nitro and azo groups.

Unit 3: Stereochemistry of Organic Compounds (18 Hrs)

3.1 Introduction to molecular symmetry and chirality: examples from common objects to molecules. Axis, plane, center, alternating axis of symmetry.

3.2 Center of chirality: molecules with C, N, S based chiral centers, absolute configuration, enantiomers, racemic modifications, R and S nomenclature using Cahn-Ingold-Prelog rules, molecules with a chiral center and Cn, molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro, threo nomenclature.

3.3 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls, ansa and cyclophanic compounds, spiranes, exo-cyclic alkylidenecycloalkanes.

3.4 Topicity and prostereoisomerism, topicity of ligands and faces as well as their nomenclature. NMR distinction of enantiotopic/diastereotopic ligands.

3.5 Stereoisomerism: definition based on symmetry and energy criteria, configuration and conformational stereoisomers.

3.6 Geometrical isomerism: nomenclature, E-Z notation, methods of determination of geometrical isomers. Interconversion of geometrical isomers.

Unit 4: Conformational Analysis (18 Hrs)

4.1 Conformational descriptors - factors affecting conformational stability of molecules. Conformational analysis of acyclic and cyclic systems: substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, congressane, sucrose and lactose. Fused and bridged bicyclic systems. Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination-Saytzeff and Hofmann eliminations), substitution and oxidation of 2^0 alcohols. Chemical consequence of conformational equilibrium - Curtin Hammett principle.

References

01. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanisms, Academic Press, 2002.

02. F.A. Carey, R. A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edn., Springer, 2007.

03. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.

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PH1C03 QUANTUM CHEMISTRY AND GROUP THEORY

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Postulates of Quantum Mechanics (9 Hrs)

1.1 State function or wave function postulate: Born interpretation of the wave function, well behaved functions, orthonormality of wave functions.

1.2 Operator postulate: operator algebra, linear and nonlinear operators, Laplacian operator, commuting and noncommuting operators, Hermitian operators and their properties, eigen functions and eigen values of an operator.

1.3 Eigen value postulate: eigen value equation, eigen functions of commuting operators.

1.4 Expectation value postulate.

1.5 Postulate of time-dependent Schrödinger equation, conservative systems and time-independent Schrödinger equation.

Unit 2: Application to Exactly Solvable Model Problems (18 Hrs)

2.1 Translational motion: free particle in one-dimension, particle in a one-dimensional box with infinite potential walls, particle in a one-dimensional box with finite potential walls-tunneling, particle in a three dimensional box-separation of variables, degeneracy.

2.2 Vibrational motion: one-dimensional harmonic oscillator (complete treatment), Hermite equation(solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features, Harmonic oscillator model and molecular vibrations.

2.3 Rotational motion: co-ordinate systems, cartesian, cylindrical polar and spherical polar coordinates and their relationships. The wave equation in spherical polar coordinates-particle on a ring, the phi equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere)-separation of variables, the phi and the theta equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms)-polar diagrams of spherical harmonics.

2.4 Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (L_x, L_y, L_z and L^2)-commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators L_z and L^2. Ladder operator method for angular momentum. Space quantization.

Unit 3: Quantum Mechanics of Hydrogen-like Atoms (9 Hrs)

3.1 Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates: separation of variables-R, theta and phi equations and their solutions, wave functions and energies of hydrogen-like atoms. Orbitals-radial functions, radial distribution functions, angular functions and their plots.

3.2 The postulate of spin by Uhlenbeck and Goudsmith, discovery of spin-Stern Gerlach experiment. Spin orbitals-construction of spin orbitals from orbitals and spin functions.

Unit 4: Symmetry and Groups (9 Hrs)

4.1 Symmetry elements, symmetry operations, point groups and their symbols, sub groups, classes, abelian and cyclic groups, group multiplication tables-classes in a group and similarity transformation.

4.2 Symmetry in crystals-32 crystallographic point groups (no derivation), Hermann-Mauguin symbols. Screw axis-pitch and fold of screw axis. Glide planes. Space groups-determination of space group symbols of triclinic and monoclinic systems.

Unit 5: Theory of Molecular Symmetry (18 Hrs)

5.1 Matrices: addition and multiplication of matrices, inverse and orthogonal matrices, character of a matrix, block diagonalisation, matrix representation of symmetry operations, representation of groups by matrices, construction of representation using vectors and atomic orbitals as basis, representation generated by cartesian coordinates positioned on the atoms of a molecule (H_2O and SO_2 as examples).

5.2 Reducible and irreducible representations-construction of irreducible representation by standard reduction formula. Statement of Great Orthogonality Theorem (GOT). Properties of irreducible representations. Construction of irreducible representation using GOT-construction of character tables for C_{2v}, C_{2h}, C_{3v} and C_{4v}. Direct product of representations.

5.3 Molecular dissymmetry and optical activity.

Unit 6: Application of Group Theory in Spectroscopy (9 Hrs)

6.1 Applications in vibrational spectra: symmetry aspects of molecular vibrations, vibrations of polyatomic molecules-selection rules for vibrational absorption. Complementary character of IR and Raman spectra-determination of the number of active IR and Raman lines.

6.2 Application in electronic spectra: electronic spectra of diatomic molecules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, types of electronic transitions, Fortrat diagram, dissociation and pre dissociation, calculation of heat of dissociation.

References

01. I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education Inc., 2009.
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17. A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010

PH1C04 CLASSICAL AND STATISTICAL THERMODYNAMICS

Credit: 3 **Contact Lecture Hours- 54**

Unit 1: Classical Thermodynamics (27 Hrs)

1.01 Entropy, dependence of entropy on variables of a system (S,T and V; S,T and P). Thermodynamic equations of state. Irreversible processes - Clausius inequality.

1.02 Free energy, Maxwell relations and significance, temperature dependence of free energy - Gibbs Helmholtz equation, applications of Gibbs Helmholtz equation.

1.03 Partial molar quantities, chemical potential and Gibbs-Duhem equations, determination of partial molar volume and enthalpy.

1.04 Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas, variation of fugacity with temperature and pressure. Activity, dependence of activity on temperature and pressure.

1.05 Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law, excess thermodynamic functions-free energy, enthalpy, entropy and volume. Determination of excess enthalpy and volume.

1.06 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- vant Hoff reaction isochore and isotherm.

1.07 Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law, entropy changes in chemical reactions.

1.08 Three component systems-graphical representation. Solid-liquid equilibria-ternary solutions with common ions, hydrate formation, compound formation. Liquid-liquid equilibria-one pair of partially miscible liquids, two pairs of partially miscible liquids, three pairs of partially miscible liquids.

1.09 Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance. Entropy production- rate of entropy production, entropy production in chemical reactions, the phenomenological relations. The principle of microscopic reversibility, the Onsager reciprocal relations. Thermal osmosis. Thermoelectric phenomena.

1.10 Bioenergetics: coupled reactions, ATP and its role in bioenergetics, high energy bond, free energy and entropy change in ATP hydrolysis, thermodynamic aspects of metabolism and respiration, glycolysis, biological redox reactions.

Unit 2: Statistical Thermodynamics (27 Hrs)

2.1 Permutation, probability, apriori and thermodynamic probability, Stirlings approximation, macrostates and microstates, Boltzmann distribution law, partition function and its physical significance, phase space, different ensembles, canonical partition function, distinguishable and indistinguishable molecules, partition function and thermodynamic functions, separation of partition function-

translational, rotational, vibrational and electronic partition functions. Thermal de-Broglie wavelength.

2.2 Calculation of thermodynamic functions and equilibrium constants, statistical interpretation of work and heat, Sakur-Tetrode equation, statistical formulation of third law of thermodynamics, thermodynamic probability and entropy, residual entropy, heat capacity of gases - classical and quantum theories, heat capacity of hydrogen.

2.3 Need for quantum statistics, Bose-Einstein statistics: Bose-Einstein distribution, example of particles, Bose-Einstein condensation, difference between first order and higher order phase transitions, liquid helium, supercooled liquids. Fermi-Dirac distribution: examples of particles, application in electron gas, thermionic emission. Comparison of three statistics.

2.4 Heat capacity of solids- the vibrational properties of solids, Einsteins theory and its limitations, Debye theory and its limitations.

References

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SEMESTER 2

PH2C05 COORDINATION CHEMISTRY

Credits: 4 **Contact Lecture Hours: 72**

Unit 1: Structural Aspects and Bonding (18 Hrs)

1.1 Classification of complexes based on coordination numbers and possible geometries. Sigma and pi bonding ligands such as CO, NO, CN^-, R_3P, and Ar_3P. Stability of complexes, thermodynamic aspects of complex formation-Irving William order of stability, chelate effect.

1.2 Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and triagonal bipyramidal fields, LFSE, *Dq* values, Jahn Teller (JT) effect, theoretical failure of crystal field theory, evidence of covalency in the metal-ligand bond, nephelauxetic effect, ligand field theory, molecular orbital theory-M.O energy level diagrams for octahedral and tetrahedral complexes without and with π-bonding, experimental evidences for pi-bonding.

Unit 2: Spectral and Magnetic Properties of Metal Complexes (18 Hrs)

2.1 Electronic Spectra of complexes-Term symbols of d^n system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for d^n and d^{10-n} ions in octahedral and tetrahedral fields (qualitative approach), *d-d* transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling.

2.2 Interpretation of electronic spectra of complexes-Orgel diagrams, demerits of Orgel diagrams, Tanabe-Sugano diagrams, calculation of *Dq*, *B* and β (Nephelauxetic ratio) values, spectra of complexes with lower symmetries, charge transfer spectra, luminescence spectra.

2.3 Magnetic properties of complexes-paramagnetic and diamagnetic complexes, molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment. Temperature dependence of magnetism-Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP), Spin state cross over, Antiferromagnetism-inter and intramolecular interaction. Anomalous magnetic moments.

2.4 Elucidating the structure of metal complexes (cobalt and nickel complexes) using electronic spectra, IR spectra and magnetic moments.

Unit 3: Kinetics and Mechanism of Reactions in Metal Complexes (18 Hrs)

3.1 Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes, *trans* effect-theory and applications.

3.2 Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic).

3.3 Electron transfer reactions: outer sphere mechanism-Marcus theory, inner sphere mechanism-Taube mechanism.

Unit 4: Stereochemistry of Coordination Compounds (9 Hrs)

4.1 Geometrical and optical isomerism in octahedral complexes, resolution of optically active complexes, determination of absolute configuration of complexes by ORD and circular dichroism, stereoselectivity and conformation of chelate rings, asymmetric synthesis catalyzed by coordination compounds,

4.2 Linkage isomerism-electronic and steric factors affecting linkage isomerism. Symbiosis-hard and soft ligands, Prussian blue and related structures, Macrocycles-crown ethers.

Unit 5: Coordination Chemistry of Lanthanides and Actinides (9 Hrs)

5.1 General characteristics of lanthanides-Electronic configuration, Term symbols for lanthanide ions, Oxidation state, Lanthanide contraction. Factors that mitigate against the formation of lanthanide complexes. Electronic spectra and magnetic properties of lanthanide complexes. Lanthanide complexes as shift reagents.

5.2 General characteristics of actinides-difference between *4f* and *5f* orbitals, comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra and magnetic properties.

References

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02. J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.

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PH2C06 ORGANIC REACTION MECHANISM

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Review of Organic Reaction Mechanisms (9 Hrs)

1.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (SN_1, SN_2, SN_i, SE_1, SE_2, addition-elimination and elimination-addition sequences), elimination (E_1 and E_2) and addition reactions (regioselectivity: Markovnikov's addition-carbocation mechanism, anti-Markovnikov's addition-radical mechanism). Elimination vs substitution.

1.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent and neighbouring group on nucleophilic substitution(SN_2 and SN_1) and elimination (E_1 and E_2) reactions.

Unit 2: Chemistry of Carbanions (9 Hrs)

2.1 Formation, structure and stability of carbanions. Reactions of carbanions: C-X bond (X = C, O, N) formations through the intermediary of carbanions. Chemistry of enolates and enamines. Kinetic and Thermodynamic enolates- lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates.

2.2 Nucleophilic additions to carbonyls groups. Named reactions under carbanion chemistry-mechanism of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorski rearrangement.

2.3 Ylids: chemistry of phosphorous and sulphur ylids - Wittig and related reactions, Peterson olefination.

Unit 3: Chemistry of Carbocations (9 Hrs)

3.1 Formation, structure and stability of carbocations. Classical and non-classical carbocations.

3.2 C-X bond (X = C, O, N) formations through the intermediary of carbocations. Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol, Dienone-phenol and Benzilic acid rearrangements, Noyori annulation, Prins reaction.

3.3 C-C bond formation involving carbocations: oxymercuration, halolactonisation.

Unit 4: Carbenes, Carbenoids, Nitrenes and Arynes (9 Hrs)

4.1 Structure of carbenes (singlet and triplet), generation of carbenes, addition and insertion reactions.

4.2 Rearrangement reactions of carbenes such as Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition.

4.3 Structure, generation and reactions of nitrene and related electron deficient nitrene intermediates.

4.4 Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.

4.5 Arynes: generation, structure, stability and reactions. Orientation effect-amination of haloarenes.

Unit 5: Radical Reactions (9 Hrs)

5.1 Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter & intramolecular) for C-C bond formation - Baldwin's rules (b) fragmentation and rearrangements-Hydroperoxide: formation, rearrangement and reactions. Autooxidation.

5.2 Named reactions involving radical intermediates: Barton deoxygenation and decarboxylation, McMurry coupling.

Unit 6: Chemistry of Carbonyl Compounds (9 Hrs)

6.1 Reactions of carbonyl compounds: oxidation, reduction (Clemmensen and Wolf-Kishner), addition (addition of cyanide, ammonia, alcohol) reactions, Cannizzaro reaction, addition of Grignard reagent. Structure and reactions of α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition-Michael addition, Mannich reaction, Robinson annulation.

Unit 7: Concerted reactions (18 Hrs)

7.1 Classification: electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions. Woodward Hoffmann rules - frontier orbital and orbital symmetry correlation approaches - PMO method.

7.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Wittig, Mislow-Evans and Sommelet-Hauser rearrangements. Diels-Alder and Ene reactions (with stereochemical aspects), dipolar cycloaddition(introductory).

7.3 Unimolecular pyrolytic elimnination reactions: cheletropic elimination, decomposition of cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides, acetates and xanthates.

7.4 Problems based on the above topics.

References

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02. F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5th Edn., Springer, 2007.

03. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 2005.

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05. A. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, 1976.

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PH2C07 CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Approximate Methods in Quantum Mechanics (18 Hrs)

1.1 Many-body problem and the need of approximation methods, independent particle model. Variation method, variation theorem with proof, illustration of variation theorem using the trial function x(a-x) for particle in a 1D-box and using the trial function e^{-ar} for the hydrogen atom, variation treatment for the ground state of helium atom.

1.2 Perturbation method, time-independent perturbation method (non-degenerate case only), first order correction to energy and wave function, illustration by application to particle in a 1D-box with slanted bottom, perturbation treatment of the ground state of the helium atom. Qualitative idea of Hellmann-Feynman theorem.

1.3 Hartree Self-Consistent Field method. Spin orbitals for many electron atoms-symmetric and antisymmetric wave functions. Pauli's exclusion principle. Slater determinants. Qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method. Roothan's concept of basis functions, Slater type orbitals (STO) and Gaussian type orbitals (GTO), sketches of STO and GTO.

Unit 2: Chemical Bonding (18 Hrs)

2.1 Schrödinger equation for molecules. Born-Oppenheimer approximation. Valence Bond (VB) theory, VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2.

2.2 Molecular Orbital (MO) theory, MO theory of H_2^+ ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules Li_2, Be_2, N_2, O_2 and F_2 and hetero nuclear diatomic molecules LiH, CO, NO and HF. Bond order. Correlation diagrams, non-crossing rule. Spectroscopic term symbols for diatomic molecules. Comparison of MO and VB theories.

2.3 Hybridization, quantum mechanical treatment of sp, sp^2 and sp^3 hybridisation. Semiempirical MO treatment of planar conjugated molecules, Hückel Molecular Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene. Calculation of charge distributions, bond orders and free valency.

Unit 3: Applications of Group Theory in Chemical Bonding (9 Hrs)

3.1 Application in quantum mechanics, transition moment integral, vanishing of integrals.

3.2 Applications in chemical bonding, construction of hybrid orbitals with BF_3, CH_4, PCl_5 as examples. Transformation properties of atomic orbitals. Symmetry adapted linear combinations (SALC) of C_{2v}, C_{2h}, C_3, C_{3v} and D_{3h}. Jahn-Teller effect. Woodward Hoffmann rules-correlation diagram.

Unit 4: Computational Chemistry (18 Hrs)

(The units 4 and 5 have been designed to expose the students to the field of computational chemistry, which has emerged as a powerful tool in chemistry capable of supplementing and complementing experimental research. The quantities which can be calculated using computational methods, how to prepare the input to get these results and the different methods that are widely used to arrive at the results are introduced here. Detailed mathematical derivations are not expected. Though computer simulations form an important part of computational chemistry, they are not covered in this syllabus.)

4.1 Introduction: computational chemistry as a tool and its scope.

4.2 Potential energy surface: stationary point, transition state or saddle point, local and global minima.

4.3 Molecular mechanics methods: force fields-bond stretching, angle bending, torsional terms, non-bonded interactions, electrostatic interactions. Mathematical expressions. Parameterisation from experiments or quantum chemistry. Important features of commonly used force fields like MM3, MMFF, AMBER and CHARMM.

4.4 Ab initio methods: A review of Hartee-Fock method. Basis set approximation. Slater and Gaussian functions. Classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, correlation consistent basis sets.

4.5 Hartree-Fock limit. Electron correlation. Qualitative ideas on post Hartree-Fock methods-variational method, basic principles of Configuration Inetraction(CI). Perturbational methods-basic principles of Møller Plesset Perturbation Theory.

4.6 General introduction to semiempirical methods: basic principles and terminology.

4.7 Introduction to Density Functional Theory (DFT) methods: Hohenberg-Kohn theorems. Kohn-Sham orbitals. Exchange correlation functional. Local density approximation. Generalized gradient approximation. Hybrid functionals (only the basic principles and terms need to be introduced).

4.8 Model Chemistry-notation, effect on calculation time (cost).

4.9 Comparison of molecular mechanics, ab initio, semiempirical and DFT methods.

Unit 5: Computational Chemistry Calculations (9 Hrs)

5.1 Molecular geometry input-cartesian coordinates and internal coordinates, Z-matrix. Z-matrix of: single atom, diatomic molecule, non-linear triatomic

molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane, ethane and butane. General format of GAMESS / Firefly input file. GAMESS / Firefly key word for: basis set selection, method selection, charge, multiplicity, single point energy calculation, geometry optimization, constrained optimization and frequency calculation.

5.2 Identifying a successful GAMESS/ Firefly calculation-locating local minima and saddle points, characterizing transition states, calculation of ionization energies, Koopmans' theorem, electron affinities and atomic charges.

5.3 Identifying HOMO and LUMO-visualization of molecular orbitals and normal modes of vibrations using suitable graphics packages.

References

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03. R.K. Prasad, Quantum Chemistry, 3rd Edn., New Age International, 2006.

04. F.A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern, 1990.

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14. C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John Wiley & Sons, 2004.

15. D.C. Young, Computational Chemistry: Practical Guide for Applying Techniques to Real-World Problems, John Wiley & Sons, 2001.

Softwares

Molecular Mechanics:

1. **Arguslab** available from www.arguslab.com/
2. **Tinker** available from www.dasher.wustl.edu/ffe/

Ab initio, semiempirical and dft:

1. **Firefly / PC GAMESS** available from http://classic.chem.msu.su/gran/gamess/
2. **WINGAMESS** available from http://www.msg.ameslab.gov/gamess/

Graphical User Interface (GUI):

1. **Gabedit** available from http://gabedit.sourceforge.net/
2. **wxMacMolPlt** available from http://www.scl.ameslab.gov/MacMolPlt/
3. **Avogadro** from http://avogadro.openmolecules.net/wiki/Get_Avogadro

PH2C08 MOLECULAR SPECTROSCOPY

Credit: 3 **Contact Lecture Hours: 54**

Unit 1: Foundations of Spectroscopic Techniques (27 Hrs)

1.1 Origin of spectra: origin of different spectra and the regions of the electromagnetic spectrum, intensity of absorption, influencing factors, signal to noise ratio, natural line width, contributing factors, Doppler broadening, Lamb dip spectrum, Born Oppenheimer approximation, energy dissipation from excited states (radiative and non radiative processes), relaxation time.

1.2 Microwave spectroscopy: principal moments of inertia and classification (linear, symmetric tops, spherical tops and asymmetric tops), selection rules, intensity of rotational lines, relative population of energy levels, derivation of J_{max} , effect of isotopic substitution, calculation of intermolecular distance, spectrum of non rigid rotors, rotational spectra of polyatomic molecules, linear and symmetric top molecules, Stark effect and its application, nuclear spin and electron spin interaction, chemical analysis by microwave spectroscopy.

1.3 Infrared spectroscopy: Morse potential energy diagram, fundamentals, overtones and hot bands, determination of force constants, diatomic vibrating rotator, break down of the Born-Oppenheimer approximation, effect of nuclear spin, vibrational spectra of polyatomic molecules, normal modes of vibrations, combination and difference bands, Fermi resonance, finger print region and group vibrations, effect of H-bonding on group frequency, disadvantages of dispersive IR, introduction to FT spectroscopy, FTIR.

1.4 Raman spectroscopy: scattering of light, polarizability and classical theory of Raman spectrum, rotational and vibrational Raman spectrum, complementarities of Raman and IR spectra, mutual exclusion principle, polarized and depolarized Raman lines, resonance Raman scattering and resonance fluorescence.

1.5 Electronic spectroscopy: term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method, electronic spectra of polyatomic molecules, spectra of transitions localized in a bond or group, free electron model, different types of lasers-solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers, introduction to UV and X-ray photoelectron spectroscopy.

Unit 2: Resonance Spectroscopy (27 Hrs)

2.1 NMR spectroscopy : interaction between nuclear spin and applied magnetic field, nuclear energy levels, population of energy levels, Larmor precession, relaxation methods, chemical shift, representation, examples of AB, AX and AMX types, exchange phenomenon, factors influencing coupling, Karplus relationship.

2.2 FTNMR, second order effects on spectra, spin systems (AB, AB_2), simplification of second order spectra, chemical shift reagents, high field NMR, double irradiation, selective decoupling, double resonance, NOE effect, two dimensional NMR, COSY and HETCOR, ^{13}C NMR, natural abundance, sensitivity, ^{13}C chemical shift and structure correlation, introduction to solid state NMR, magic angle spinning.

2.3 EPR spectroscopy: electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, determination of g values ($g_{||}$ and $g_{\perp}$), fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.

2.4 An elementary study of NQR spectroscopy.

2.5 Mossbauer spectroscopy: principle, Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift, application to metal complexes, MB spectra of Fe(II) and Fe(III) cyanides.

References

01. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.

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SEMESTERS 1 AND 2

PH2P01 INORGANIC CHEMISTRY PRACTICAL

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

Separation and identification of two less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li. Anions which need elimination not to be given. Minimum eight mixtures to be given.

PART II

Colorimetric estimation of Fe, Cu, Ni, Mn, Cr, NH_4^+, nitrate and phosphate ions.

PART III

Preparation and characterization complexes using IR, NMR and electronic spectra.

(a) Tris (thiourea)copper(I) complex

(b) Potassium tris (oxalate) aluminate (III).

(c) Hexammine cobalt (III) chloride.

(d) Tetrammine copper (II) sulphate.

(e) Schiff base complexes of various divalent metal ions.

References

01. A.I. Vogel, G. Svehla, Vogel's Qualitative Inorganic Analysis, 7th Edn., Longman,1996.

02. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman,1966.

03. I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn., Mc Millian, 1968.

04. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National Pub.Co., 1974.

PH2P02 ORGANIC CHEMISTRY PRACTICAL

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

General methods of separation and purification of organic compounds such as:

1. Solvent extraction
2. Soxhlet extraction
3. Fractional crystallization
4. TLC and Paper Chromatography
5. Column Chromatography
6. Membrane Dialysis

PART II

1. Separation of Organic binary mixtures by chemical/solvent separation methods
2. Separation of organic mixtures by TLC
3. Separation/ purification of organic mixtures by column chromatography

PART III

Drawing the structures of organic molecules and reaction schemes by ChemDraw, Symyx Draw and Chemsketch. Draw the structures and generate the IR and NMR spectra of the substrates and products in the following reactions:

1. Cycloaddition of diene and dienophile (Diels-Alder reaction)
2. Oxidation of primary alcohol to aldehyde and then to acid
3. Benzoin condensation
4. Esterification of simple carboxylic acids
5. Aldol condensation

References

01. A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

02. A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.

03. F.G. Mann, B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.

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PH2P03 PHYSICAL CHEMISTRY PRACTICAL

Credit: 3 **Contact Lab Hours: 72+72 =144**

(One question each from both parts A and B will be asked for the examination)

Part A

I. Adsorption

1. Verification of Freundlich and Langmuir adsorption isotherm: charcoal-acetic acid or charcoal-oxalic acid system.
2. Determination of the concentration of the given acid using the isotherms.

II. Phase diagrams

1. Construction of phase diagrams of simple eutectics.
2. Construction of phase diagram of compounds with congruent melting point: diphenyl amine-benzophenone system.
3. Effect of (KCl/succinic acid) on miscibility temperature.
4. Construction of phase diagrams of three component systems with one pair of partially miscible liquids.

III. Distribution law

1. Distribution coefficient of iodine between an organic solvent and water.
2. Distribution coefficient of benzoic acid between benzene and water.
3. Determination of the equilibrium constant of the reaction $KI + I_2 \leftrightarrow KI_3$

IV. Surface tension

1. Determination of the surface tension of a liquid by
   a) Capillary rise method
   b) Drop number method
   c) Drop weight method
2. Determination of parachor values.
3. Determination of the composition of two liquids by surface tension measurements

Part B

Computational chemistry experiments

V. Experiments illustrating the capabilities of modern open source/free computational chemistry packages in computing single point energy, geometry optimization, vibrational frequencies, population analysis, conformational studies, IR and Raman spectra, transition state search, molecular orbitals, dipole moments etc.

Geometry input using Z-matrix for simple systems, obtaining Cartesian coordinates from structure drawing programs like Chemsketch.

References

01. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.

02. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.

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04. GAMESS documentation available from: http://www.msg.ameslab.gov/gamess/documentation.html

SEMESTER 3

PH3C09 SYNTHETIC AND BIOORGANIC CHEMISTRY

Credit : 4 **Contact Lecture Hours: 72**

Unit 1: Organic Synthesis via Oxidation and Reduction (18 Hrs)

1.1 Survey of organic reagents and reactions in organic chemistry with special reference to oxidation. Metal based and non-metal based oxidations of (a) alcohols to carbonyls (chromium, manganese, aluminium, and silver based reagents) (b) phenols (Fremy's salt, silver carbonate) (c) alkenes to epoxides (peroxides/peracids based), Sharpless asymmetric epoxidation.(d) alkenes to diols (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction. (e) alkenes to carbonyls with bond cleavage (manganese, osmium, ruthenium and lead based, ozonolysis) (f) alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation) (g) ketones to ester/lactones (Baeyer-Villiger).

1.2 Survey of organic reagents and reactions in organic chemistry with special reference to reduction:(a) Catalytic hydrogenation (Heterogeneous: Pd /Pt /Rh / Ni etc; Homogeneous: Wilkinson). Noyori asymmetric hydrogenation. (b) Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium and Zinc (Birch, Pinacol formation, McMurry, Acyloin formation, dehalogenation and deoxygenations) (c) Hydride transfer reagents from Group III and Group IV in reductions. (i) $NaBH_4$ triacetoxyborohydride; $LiAlH_4$ and DIBAL-H, Meerwein-Pondorff-Verley reduction) (ii) Stereo/enantioselective reductions (Chiral Boranes, Corey-Bakshi-Shibata).

1.3 Problems based on the above topics.

Unit 2: Modern Synthetic Methods (9 Hrs)

2.1 Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Ugi reaction. Brook rearrangement. Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann. Directed ortho metalation.

2.2 Problems based on the above topics.

Unit 3: Stereoselective Transformations (9 Hrs)

3.1 Stereoselective synthesis of tri- and tetra-substituted olefins. Synthetic applications of Claisen rearrangement and its variants, aza-Cope rearrangement (Overman rearrangement), ene reaction (metallo-ene; Conia ene), Prins reaction. Asymmetric synthesis.

3.2 Problems based on the above topics.

Unit 4: Construction of Ring Systems (9 Hrs)

4.1 Different approaches towards the synthesis of three, four, five and six-membered rings.

4.2 Photochemical approaches for the synthesis of four membered rings, oxetanes and cyclobutanes. Diels-Alder reaction (inter and intra molecular), ketene cycloaddition (inter and intra molecular), Pauson-Khand reaction, Bergman cyclization, Nazarov cyclization, cation-olefin cyclization and radical-olefin cyclization.

4.3 Inter-conversion of ring systems (contraction and expansion), construction of macrocyclic rings, ring closing metathesis.

4.4 Problems based on the above topics.

Unit 5: Molecular Recognition and Supramolecular Chemistry (9 Hrs)

5.1 Concept of molecular recognition, host-guest complex formation, Forces involved in molecular recognition.

5.2 Molecular receptors: Cyclodextrins, Crown ethers, Cryptands, Tweezers, Carcerands, Cyclophanes, Calixaranes, carbon nanocapsules.

5.3 Importance of molecular recognition in biological systems, Controlled release phenomena.

5.4 Applications of Supramolecular complexes in medicine and perfumery industries.

Unit 6: Chemistry of Natural Products and Biomolecule (18 Hrs)

6.1 Steroids: classification and nomenclature of steroids. Reactions, structure elucidation, stereochemistry and biosynthesis of cholesterol. Structure and semi synthesis of steroid hormones-testosterone, estrogen and progesterone. Biosynthesis of steroids.

6.2 Alkaloids: General methods of structure elucidation of alkaloids. Structure elucidation and synthesis of papaverine, quinine and morphine. Stereoselctive synthesis of reserpine. Biosynthesis of alkaloids.

6.3 Vitamines: classification, structure and synthesis of vitamins A, C, B_1 and B_2.

6.4 β-lactam antibiotics: structures of pencillins and cephalosphorins, synthesis of pencillins and chloramphenicol.

6.5 Natural colouring species: anthocyanins and carotenoids, structure and synthesis of cyanin, flavone, quercetine and β-carotene.

References

01. F.A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2009.

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13. J.W. Steed, J.L. Atwood, Supramolecular Chemistry, John Wiley & Sons, 2009.

14. H. Dodziuk, Introduction to Supramolecular Chemistry, Springer, 2002.

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16. R.C. Larock, Comprehensive Organic Transformations, VCH, 1989.

PH3C10 PHYSICAL CHEMISTRY

Credit : 4 **Contact Lecture Hours: 72**

Unit 1: Chemical Kinetics (18 Hrs)

1.1 Theories of reaction rates: Collision theory-steric factor, potential energy surfaces. Conventional transition state theory-Eyring equation. Comparison of the two theories. Thermodynamic formulation of the two theories. Thermodynamic formulation of the reaction rates. Significance of $\Delta G^{\neq}$, $\Delta H^{\neq}$ and $\Delta S^{\neq}$. Volume of activation. Effect of pressure and volume on velocity of gas reactions.

1.2 Lindemamann-Hinshelwood mechanism and RRKM theory of unimolecular reactions. Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation, Hammet and Taft equation, kinetic isotope effect.

1.3 Fast reactions: relaxation, flow and shock methods, flash photolysis, NMR and ESR methods of studying fast reactions.

1.4 Acid-base catalysis: specific and general catalysis, Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanism with examples, acidity function.

1.5 Enzyme catalysis and its mechanism, Michelis-Menten equation, effect of pH and temperature on enzyme catalysis.

1.6 Kinetics of enzyme inhibition, protein folding and pathological misfolding, muscle contraction and molecular motors.

Unit 2: Surface Chemistry and Colloids (18 Hrs)

2.1 Different types of surfaces, thermodynamics of surfaces, Gibbs adsorption equation and its verification, surfactants and micelles, general properties of emulsions, foam structure, aerosols, surface films, surface pressure and surface potential and their measurements and interpretation. Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy, ion scattering, SEM and TEM in the study of surfaces.

2.2 Adsorption: The Langmuir theory, kinetic and statistical derivation, multilayer adsorption-BET theory, Use of Langmuir and BET isotherms for surface area determination. Application of Langmuir adsorption isotherm in surface catalysed reactions, the Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism, flash desorption.

2.3 Colloids: Zeta potential, electrokinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium.

Unit 3: Photochemistry **(18 Hrs)**

3.1 Quantum yield, chemical actinometry, excimers and exciplexes, photosensitization, chemiluminescence, bioluminescence, thermoluminescence, pulse radiolysis, hydrated electrons, photostationary state, dimerisation of anthracene, ozone layer in the atmosphere, chemistry of photosynthesis, photography and vision.

3.2 Principle of utilization of solar energy, solar cells and their working.

3.3 Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type, effect of temperature on emissions, photochemistry of environment, green house effect, two photon absorption spectroscopy, application of pulsed laser in measuring the dynamics of photochemical processes. Photochemistry of vision. Phototaxis and phototropism. Photochemistry of nucleic acids. Vitamin D

.

Unit 4: Nanotechnology and Green Chemistry **(18 Hrs)**

5.1 Basic principles of nanochemistry, methods of synthesis of nanomaterials, a brief study of carbon nanotubes, fullerenes, quantum dots and metal nanoparticles. Applications of nanomaterials in medicine: immunogold labelling, applications in medical diagnosis, nanobased drug delivery, biomimetic nanotechnology, DNA nanotechnology and structural biomimicry.

5.2 Principles of green chemistry, basic concepts, atom economy, twelve laws of green chemistry, principles of green organic synthesis.

5.3 Green alternatives of organic synthesis: coenzyme catalysed reactions, green alternatives of molecular rearrangements, electrophilic aromatic substitution reactions, oxidation-reduction reactions, clay catalysed synthesis, condensation reactions. Green photochemical reactions. Microwave assisted organic synthesis.

5.4 Green chemistry in the pharmaceutical industry: Ibuprofen manufacture, biocatalysis.

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17. R. Ballini, Eco-Friendly Synthesis of Fine Chemicals, RSC, 2009.

PH3C11 DRUG DESIGN AND PHARMACOLOGY

Credit : 4 **Contact Lecture Hours: 72**

Unit 1: Principles of Drug Therapy and Drug Design (18 Hrs)

1.1 General Principles of Drug Therapy. Relationship between chemical structure, lipid solubility and biological activity of drugs. Stereochemistry and biological activity.

1.2 Drug action-receptor theories. Drug metabolism–different pathways.

1.3 Drug design: various factors of drug design, rational drug design. Methods of lead discovery: optimisation of the lead, natural and synthetic sources of lead compounds. Bioisosterism. Prodrug and soft drug concept. Drug synthesis. Combinatorial synthesis (basic concepts). Retrosynthetic analysis of benzocaine, saccharin, salbutamol and benzodiazepines.

1.4 Basic concepts of CADD, molecular modeling, molecular docking. QSAR-physicochemical parameters, introduction to 2D & 3D QSAR.

Unit 2: Pharmacology (9 Hrs)

2.1 General principles of pharmacology: biological response to drugs, passage of drugs across membranes.

2.2 Pharmacokinetic principles: absorption, distribution, metabolism and excretion of drugs. Dose of drugs and routes of administration.

2.3 Pharmacodynamic principles: dose response relationships, mechanism of drug action, unusual and adverse responses of drugs, structurally specific and nonspecific drugs. Ferguson's principle.

2.4 Drug interactions-synergism, antagonism, drug addiction and drug dependence, drug tolerance, drug hypersensitivity.

Unit 3: Metallic compounds used in pharmaceutical chemistry (9 Hrs)

3.1 Calcium lactate, calcium gluconate, iron gluconate, iron fumerate, ferric ammonium citrate, ferrous sulphate, aluminium hydroxide gel, calamin, zinc oxide, zinc stearate, magnesium stearate, talc, yellow mercuric oxide, trivalent and pentavalent antomonials, selenium sulfide, lithium salts, gold, platinum and bismuth compounds.

3.2 Metal toxicity - cadmium, lead, copper and mercury.

Unit 4: Drugs acting on CNS **(18 Hrs)**

4.1 General anaesthetics. Inhalation anaesthetics - ether, enflurane, halothane, nitrous oxide, cyclopropane. Intravenous anaesthetics - thiopentone sodium, ketamine.

4.2 Hypnotics, sedatives and anxiolytic agents.

4.3 Anxiolytic agents-benzodiazepines, buspirone and meprobamate.

4.4 Anticonvulsants: convulsions, types of epilepsy, barbiturates-hydantoins, oxazolidinediones, succinimides and benzodiazepines.

4.5 Analeptics: xanthines, amphetamines, nikethamide and ethamivan.

4.6 Centrally acting muscle relaxants: glyceryl ethers-mephenesin, alkane diol derivatives-meprobamate, benzodiazepines-librium, diazepam and baclofen.

4.7 Antiparkinson's agents: dopamine agonists, dopamine releasing agents and synthetic anticholinergics.

4.8 Drugs for Alzheimer's disease: cholinergic agonists and acetylcholine esterase inhibitors.

4.9 Synthesis of the following drugs - Enflurane, Ketamine,Etomidate, Phenobarbital, Diazepam, Chlordiazepoxide, Meprobamate, Buspirone, Ethinamide, Nikethamide, Ethamivan, Trimethadione,Ethosuximide, Denzimol, Topiramate, Mephenesin, Levodopa, Besiperidine and Tacrine.

Unit 5: Analgesics **(9 Hrs)**

5.1 Narcotic analgesics - morphine and its analogues, phenyl(ethyl) piperidines, diphenyl heptanones and benzocaine derivatives.

5.2 Antipyretics and NSAIDs: Basic idea of COX I &I I inhibitors, salicylates-aspirin, p-aminophenol derivatives-paracetamol, phenacetin, pyrazolidinediones-phenyl butazone, oxyphenbutazone, anthranilicacid derivatives-mefanamic acid, flufenamic acid,indoleacetic acid derivatives-indomethacin, arylacetic/propionic acid derivatives(ibuprofen, ketoprofen, flubiprofen and diclofenac), oxicams(piroxicam and tenoxicam).

5.3 Drugs used for gout - allopurinol, selective COX II inhibitors

5.4 Synthesis of the following drugs-levorphanol, pethidine, methadone, phenyl butazone, flufenamic acid, diclofenac, piroxicam, allopurinol and celicoxib.

References

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02. T. Nogrady, D.F. Weaver, Medicinal Chemistry, Oxford University Press, 2005.

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PH3C12 SPECTROSCOPIC METHODS IN CHEMISTRY

Credit : 3 **Contact Lecture Hours: 54**

Unit 1: Ultraviolet-Visible and Chirooptical Spectroscopy (9 Hrs)

1.1 Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules.

1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions. Chirooptical properties-ORD, CD, octant rule, axial haloketone rule, Cotton effect.

1.3 Problems based on the above topics.

Unit 2: Infrared Spectroscopy (9 Hrs)

2.1 Fundamental vibrations, characteristic regions of the spectrum (fingerprint and functional group regions), influence of substituent, ring size, hydrogen bonding, vibrational coupling and field effect on frequency, determination of stereochemistry by IR technique.

2.2 IR spectra of C=C bonds(olefins and arenes) and C=O bonds.

2.3 Problems on spectral interpretation with examples.

Unit 3: Nuclear Magnetic Resonance Spectroscopy (18 Hrs)

3.1 Magnetic nuclei with special reference to ^{1}H and ^{13}C nuclei. Chemical shift and shielding/deshielding, factors affecting chemical shift, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. Proton and ^{13}C NMR scales.

3.2 Spin-spin splitting: AX, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling, first order and non-first order spectra, Pascal's triangle, coupling constant, mechanism of coupling, Karplus curve, quadrupole broadening and decoupling, diastereomeric protons, virtual coupling, long range coupling-epi, peri and bay effects. NOE. NOE and cross polarization.

3.3 Simplification non-first order spectra to first order spectra: shift reagents, , spin decoupling and double resonance, off resonance decoupling. Chemical shifts and homonuclear/heteronuclear couplings. Basis of heteronuclear decoupling.

3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY

3.5 Polarization transfer. Selective Population Inversion. DEPT, INEPT and RINEPT. Sensitivity enhancement and spectral editing, MRI.

3.6 Problems on spectral interpretation with examples.

Unit 4: Mass Spectrometry **(9 Hrs)**

4.1 Molecular ion: ion production methods (EI). Soft ionization methods: SIMS, FAB, CA, MALDI, PD, Field Desorption Electrospray Ionization. Fragmentation patterns-nitrogen and ring rules. McLafferty rearrangement and its applications. HRMS, MS-MS, LC-MS, GC-MS.

4.2 Problems on spectral interpretation with examples.

Unit 5: Structural Elucidation Using Spectroscopic Techniques **(9 Hrs)**

5.1 Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, ^{1}HNMR and ^{13}CNMR spectroscopy (HRMS data or Molar mass or molecular formula may be given).

5.2 Interpretation of the given UV-Vis, IR and NMR spectra.

References

01. D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3rd Edn., Brooks Cole, 2000.

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11. E.B. Wilson Jr., J.C. Decius, P.C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover Pub., 1980.

12. Online spectral databases including RIO-DB.

SEMESTER 4

ELECTIVE COURSES

(Any 3 courses to be opted from the following courses)

PH4E01 BACTERIOLOGY AND BIOCHEMISTRY

Credit : 4 **Contact Lecture Hours: 90**

Unit 1: Introduction to Microbiology (9 Hrs)

1.1 A general study of viruses, fungi and protozoa. Morphology, classification and scientific nomenclature of bacteria. Growth requirements of bacteria and nutrient media. Staining of bacteria, theories of staining. General principles of microbial control- sterilization and disinfection.

Unit 2: Immunity (9 Hrs)

2.1 Types of immunity. Antigens and antibodies: theories of antigen-antibody reactions, applications of antigen-antibody reactions. Interferons. Vaccines and sera - general study of the preparation of different types of vaccines, sera and toxoids. AIDS.

Unit 3: Amino acids, Proteins and Nucleic Acids (18 Hrs)

3.1 Cells-classification and cell division.

3.2 Essential amino acids. Primary structure of proteins and amino acid analysis. Ramachandran plot and secondary structure of proteins. Tertiary structure and structural motifs-protein folding and domain structure of proteins. Quaternary structure of proteins. Purification and characterization of proteins. Functions of proteins. Chemical synthesis of proteins-protecting groups, solid phase peptide synthesis.

3.3 DNA and RNA. Double helical structure of DNA. Replication of DNA. RNA-classification of RNA. Genetic code. Nucleic acids as carriers of genetic information. Protein biosynthesis. DNA fingerprinting technique. Elementary principles of Recombinant DNA technology, gene therapy, cloning and bioinformatics.

Unit 4: Enzymes and Hormones 18 Hrs)

4.1 Nomenclature and classification of enzymes. Mechanism of enzyme action. Substrate specificity of enzymes. Enzyme inhibition. Isoenzymes. Allosteric enzymes. Enzyme synthesis. Enzymes and digestion of food. Clinical uses of

enzymes. Immobilization of enzymes. Clinical tests for sugar and cholesterol. ELIZA.

4.2 Functions and modes of actions of hormones. Pituitary, thyroid, parathyroid, pancreatic, adrenal and adrenocortical hormones. Male and female sex hormones. Antihormones.

Unit 5: Biological Oxidation and Metabolism (27 Hrs)

5.1 ATP and ADP. Oxidative phosphorylation. Cytochromes.

5.2 Food as a source of energy. Calorific value of food. Basal metabolism. Respiratory quotient.

5.3 Carbohydrate metabolism: Glycogenesis and Glycolysis. Blood sugar level. Cori cycle. The role of insulin. The citric acid cycle. Genetic and metabolic disorders. Diabetes mellitus (type 1 and type 2). Lipaemia.

5.4 Lipid metabolism. Oxidation of fatty acids. Ketogenesis and ketosis. Biosynthesis of fatty acids. Essential fatty acids. Prostaglandins-nomenclature, structure and biosynthesis.

5.5 Metabolism of amino acids and proteins. Oxidative deamination and trans amination reactions. Urea formation-ornithine cycle. Inborn errors of metabolism.

Unit 6: Blood Composition and Acid Base Balance (9 Hrs)

6.1 Blood groups-Rh factor. Blood transfusion. Composition of blood cells. Chemistry of haemoglobin. Anaemias. Plasma proteins. Blood clotting- factors and mechanism. Coagulants.

6.2 Regulation of acid base balance. Acidosis and alkalosis. Renal function-formation and composition of urine.

References

01. A.J. Salle, Fundamental Principles of Bacteriology, Tata McGraw Hill, 1984.

02. M.J. Pelczar Jr., E.C.S. Chan, N.R. Krieg, Microbiology, 88th Edn., Tata McGraw Hill, 1993.

03. G.G. Young, Witton's Microbiology, Literacy Licensing, LLC, 2011.

04. L. Prescott, J. Harley, D. Klein, Microbiology, 6th Edn., McGraw Hill, 2005.

05. G. Sykes, Disinfection and Sterilization, Van Nostrand, 1958.

06. J.M. Berg, J.L. Tymoczko, L. Stryer, Biochemistry, 5th Edn., W.H. Freeman, 2002.

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PH4E02 ADVANCED PHARMACEUTICAL OPERATIONS AND DISPENSING

Credit :4 **Contact Lecture Hours: 90**

Unit 1: Pharmacognosy (27 Hrs)

1.1 Pharmacognosy of the official drugs frequently used in pharmacy: their sources and constituents. Eg:- senna, belladona, digitalis, stramonium,vasaka, cinnamon, cinchona, ergot, cannabis, ipecacuanha, rauwolfia, liquorice, ginger, cloves, pyrethrum, santonica, nutmeg, nuxvomica, cardamom, umbelliferous fruits like Cumin, Fennel, Caraway, Opium, Aloes, Asafoetida, Vinca rosea, Brammi (two varieties).

1.2 Fixed oils and essential oil used in pharmacy-their sources. Extraction, constituents, composition analysis of fixed oils. Elementary study of adulteration of fixed oils.

1.3 Fixed Oils: Castor oil, Olive oil, Shark liver oil.

1.4 Essential Oils: Eucalyptus oil, Turpentine oil.

1.5 A brief study of the substances used as pharmaceutical necessities – Starches, Gum Acacia, Gum Tragacanth, Agar Agar, Gelatin, Talc, Kaolin. Bentonite.

Unit 2: Dispensing (9 Hrs)

2.1 Principles of dispensing medicaments. Incompatibilities and its overcoming. Preparation of pills, tablets, capsules, injectables, suppositories, coating of tablets. Newer Drug Delivery systems-site specific drug delivery systems in cancer chemotherapy to brain and CNS, to GIT, to kidney and urinary tract. Implanted mechanical pumps.

Unit 3: Forensic Pharmacy (18 Hrs)

3.1 Pharmaceutical Legislation in India. Legal aspects of trade in drugs. The drug Act and Drug rules. The Pharmacy Act. The dangerous Drug Act and Rules. The Drugs and Cosmetic Act and rules

3.2 Introduction to Pharmacopeia B.P, I.P. and general standard analysis,

3.3 Intellectual Property Rights (IPR), Patents, Trademarks, Copy rights, Patent Acts-relevant sections (basic ideas only)

Unit 4: Pharmaceutical Operations (18 Hrs)

4.1 Principles involved, apparatus and machinery used in general pharmaceutical operations of IP/BP - evaporation, extraction crystallization, distillation.

4.2 Chromatographic techniques: theory of chromatography, applications of adsorption, partition, thin layer and column chromatographic methods. LC, HPLC, GC and GPC. Column matrices. Detectors. Affinity and chiral columns.

4.3 Electrophoresis - general ideas.

4.4 Solvent extraction, Liquid – liquid extraction, use of oxine. Ultra centrifugation, dithiazone - in extraction.

Unit 5: Diagnostic Agents and Tests **(18 Hrs)**

5.1 Radiopaques - organo iodo compounds. Compounds used in function tests, dyes, radio isotopes, RIA, ELISA.

5.2 Dyes used in pharmacy: fluorescein, mercurochrome, acridine dyes.

5.3 Colouring agents: official colours, colour code.

5.4 Liver and gastric function tests and kidney function tests.

References

01. T.E. Wallis, Text Book of Pharmacognosy, 5th Edn., J&A Churchil, 1967

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PH4E03 MEDICINAL CHEMISTRY

Credit : 4 **Contact Lecture Hours: 90**

Unit 1: Drugs acting on ANS (18 Hrs)

1.1 Adrenergic stimulants: Phenyl ethanolamine derivatives-adrenaline, isoprenaline, salbutamol, ephedrine, and phenylephrine. Imidazole derivatives-naphazoline, xylometazoline and oxymetazoline.

1.2 Adrenergic blockers: α and β adrenoreceptor antagonists-ergot akaloids, phenoxybenzamine, phentolamine, tolazoline, DCI, propranolol, atenolol, labetolol. Neurone blockers–Bretilium and Xylocholine.

1.3 Cholinergic stimulants: nicotinic and muscarinic receptors, acetyl choline and analogues, pilocarpine, bethanechol and carbachol.

1.4 Cholinergic blockers: tertiary and quaternary antimuscarinics, antispasmodic drugs-dicyclomine, glycopyrrolate, antiulcer drugs-pirenzepine, cycloplegic drugs-tropicamide, homatropine

1.5 Anticholinesterases: Competitive inhibitors-physostigmine and neostigmine.

1.6 Non competitive inhibitors: organophosphorus compounds, Nerve gases, Cholinesterase regenerators-2 PAM.

1.7 Ganglion blocking agents: mecamylamine and trimethophan

1.8 Curareform drugs: curare alkaloids, erythrina alkaloids and gallamine.

1.9 Synthesis of the following drugs: salbutamol, naphazoline, tolazoline, propranolol, bretilium, carbachol, mecamylamine and gallamine.

Unit 2: Drugs acting on CVS (9 Hrs)

2.1 Cardiotonic drugs: cardiac glycosides-their chemistry and stereochemistry, Digoxin and digitoxin.

2.2 Antiarrhythmic drugs: quinidine, disopyramide, lidocaine, phenytoin and procainamide, β-blockers-propranolol. Calcium channel blockers-verapamil and Neurone blockers-bretilium.

2.3 Antihypertensive Drugs: peripheral antiadrenergics-prazosin and terazosin. Centrally acting drugs-reserpine, clonidine and methyl dopa. β-blockers-propranolol, atenolol and labetalol. Calcium channel blockers-nifedipine and amlodipine. ACE inhibitors-captopri. Angiotensin receptor blockers-losartan. Diuretics-thiazide diuretics.

2.4 Antianginal drugs: vasodilators-nitrites and nitrates, β-blockers-propranolol. Calcium channel blockers-verapamil and nifedipine. Miscellaneous-dipyridamol and aspirin.

2.5 Anticoagulants: heparin, coumarin derivatives and indane dione derivatives.

2.6 Antilipidemic agents: atherosclerosis(mention only), Statins-lovastatin, simvastatin, fluvastatin, Fibrates-clofibrate, Miscellaneous-bile acid sequestrants and cholestyramine resin.

2.7 Synthesis of the following drugs: procainamide, disopyramide, amlodipine, verapamil, captopril and fluvastatin.

Unit 3: Chemotherapy (27 Hrs)

3.1 Antibiotics: β-lactam antibiotics-penicillins and cephalosporins, natural, biosynthetic and semisynthetic penicillins, tetracyclines and chloramphenicol, a brief study of macrolide antibiotics, aminoglycoside antibiotics, polyene antibiotics, fluoroquinolones.

3.2 Sulphonamides: sulphanilamide, N-substituted sulphanilamide derivatives, mechanism of action, sulphones-dapsone, dihydrofolate reductase inhibitors-trimethoprim and cotrimoxazole.

3.3 Antitubercular agents: first line drugs-isoniazid, rifampicin, pyrazinamide, ethambutol, and streptomycin. Second line drugs-ethionamide, paraaminosalicylic acid and fluoroquinolones.

3.4 Antifungal agents: Antibiotics-amphotericinB, griseofulvin and nystatin. Azole derivatives-ketoconozole,terconozole,fluconozole and clotrimazole. Pyrimidine derivatives- 5 Flucytosine.

3.5 Antiviral drugs: amantidine, interferon and ribavirin. Anti HIV agents-zidovudine, and abacavir. Anti herpes simplex agents-brivudine, vidarabin and acyclovir. Anti-influeza agents-oseltamivir(tamiflu).

3.6 Antiprotozoal agents: Amoebicides-metranidazole and tinidazole. Antimalarials-chloroquine, primaquine, mefloquine, quinacrine and proguanil. Anthelmintics-piperazines and benzimidazoles. Miscellaneous-eflornithine and pentamidine. Synthesis of the following drugs: ampicillin, cephalexin, chloramphenicol, sulphamethoxazole, dapsone, trimethoprim, ethambutol, griseofulvin, clotrimazole, acyclovir, metranidazole, primaquine, mebendazole.

Unit 4: Antineoplastic Drugs (9 Hrs)

4.1 Neoplasm-cause therapeutic approaches. Alkylating agents-nitrogen mustards, nitrosourea, aziridines and aryl sulphonates. Antimetabolites-folic acid. Antagonists-purine and pyrimidine antagonists. Antibiotics-anthracyclines, actinomycinD, bleomycin. Plant products-vinca alkaloids, taxol derivatives. Hormones and their antagonists-tamoxifen. Miscellaneos-procarbazine, cisplatin.

4.2 Synthesis of the following drugs: chlorambucil, carmustin, thiotepa, methotrexate, 5-fluoro uracil, procarbazine.

Unit 5: Psychopharmocological Agents (9 Hrs)

5.1 Tranquilisers: rauwolfia alkaloids, meprobamate, oxazepim, benzodiazepines, chlordiazepoxide, phenothiazene derivatives.

5.2 Antidepressants: MAO inhibitors-Isocarboxazide, tranylcypromine and phenelzine. Tricyclic compounds-imipramine, trimipramine, amitriptynine, doxepine, amoxapine. Miscellaneous compounds-fluoxetine and trazodone.

5.3 Antipsychotics: phenothiazine and thiothixene derivatives, butyrophenones-haloperidol, droperidon, rauwolfia alkaloids.

5.4 Hallucinogens: triptaminederivatives-DMT, psilocybin, phenylalkylamines-mescaline, lysergic acid derivatives-LSD.

5.5 Synthesis of the following drugs: chlordiazepoxide, meprobamate, imipramine chlorpromazine, tranylcypromine and haloperidol.

Unit 6: Miscellaneous class of compounds (18 Hrs)

6.1 Diuretics: common diuretics and their mechanism of action-mercurial and nonmercurial diuretics, carbonic anhydrase inhibitors- acetazolamide and methazolamide, thiazide derivatives-hydrochlorothiazide, Loop diuretics-furosemide and ethacrynic acid, potassium sparing diuretics-amiloride, spironolactone.

6.2 Antihistaminic drugs: histamine and its biological role, H1 antagonists-aminoalkyl ethers, diphenhydramine and doxylamine, ethylenediamine derivatives-pyrilamine, phenothiazines-promethazine, trimeprazine, piperazine derivatives-cyclizines, miscellaneous compounds-cetrizine and cyproheptadine.

6.3 Hypogycemic agents: type 1 and type 2 diabetes, insulin, suphonyl ureas-tolbutamide, acetohexamide and glibenclamide, biguanides-metformin, thiazolidinediones-rosiglitazone.

6.4 Local anaesthetics: clinical application of local anaesthesia, coca and cocaine, hexylcaine, paraaminobenzoic acid derivative-benzocaine, procaine, tetracaine, chloroprocaine, anilides, lidocaine, etiodacaine and prilocaine.

6.5 Antitussives: centrally acting antitussives-opium alkaloids and synthetic substitutes-codaine, noscapine, pholcodine, ethylmorphine, dextromethorphan, Non narcotic antitussives-diphenhydramine, expectorants-terpin hydrate, guaicol and bromhexine.

6.6 Gastrointestinal drugs: purgatives-irritant, osmotic, bulk and lubricant purgatives, Antacids-systemic and non systemic antacids, H2 antagonists-cimetidine and ranitidine, proton pump inhibitors-omeprazole and pantaprazole, digestants, carminatives and antidiarrheals.

6.7 Synthesis of the following drugs: acetazolamide, chlorthiazide furosemide, ethacrynic acid, amiloride, diphenhydramine, pyrilamine, promethazine, omeprazole, tolbutamide, phenformin, benzocaine, procaine lidocaine, dextromethorphan.

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PH4E04 ANALYTICAL CHEMISTRY

Credit : 4 **Contact Lecture Hours: 90**

Unit 1: Instrumental Methods (36 Hrs)

1.1 Electrical and nonelectrical data domains-transducers and sensors, detectors, examples for piezoelectric, pyroelectric, photoelectric, pneumatic and thermal transducers. Criteria for selecting instrumental methods - precision, sensitivity, selectivity, and detection limits.

1.2 Signals and noise: sources of noise, S/N ratio, methods of enhancing S/N ratio– hardware and software methods.

1.3 Electronics: transistors, FET, MOSFET, ICs, OPAMs. Application of OPAM in amplification and measurement of transducer signals.

1.4 UV-Vis spectroscopic instrumentation: types of optical instruments, components of optical instruments–sources, monochromators, detectors. Sample preparations. Instrumental noises. Applications in qualitative and quantitative analysis.

1.5 Molecular fluorescence and fluorometers: photoluminiscence and concentration-electron transition in photoluminescence, factors affecting fluorescence, instrumentation details. Fluorometric standards and reagents. Introduction to photoacoustic spectroscopy.

1.6 IR spectrometry: Instrumentation designs-various types of sources, monochromators, sample cell considerations, different methods of sample preparations, detectors of IR-NDIR instruments. FTIR instruments. MidIR absorption spectrometry. Determination of path length. Application in qualitative and quantitative analysis.

1.7 Raman Spectrometric Instrumentation: sources, sample illumination systems. Application of Raman Spectroscopy in inorganic, organic, biological and quantitative analysis.

1.8 NMR Spectrometry-magnets, shim coils, sample spinning, sample probes (^{1}H, ^{13}C, ^{32}P). Principle of MRI.

Unit 2: Sampling (18 hrs)

2.1 The basis and procedure of sampling, sampling statistics, sampling and the physical state, crushing and grinding, the gross sampling, size of the gross sample, sampling liquids, gas, and solids(metals and alloys), preparation of a laboratory sample, moisture in samples-essential and non-essential water, absorbed and occluded water, determination of water(direct and indirect methods).

2.2 Decomposition and dissolution, source of error, reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$, HF, microwave decompositions, combustion methods, use of fluxes like Na_2CO_3, Na_2O_2, KNO_3, NaOH, $K_2S_2O_7$,

B_2O_3 and lithium metaborate. Elimination of interference from samples-separation by precipitation, electrolytic precipitation, extraction and ion exchange. Distribution ratio and completeness of multiple extractions. Types of extraction procedures.

Unit 3: Applied Analysis **(9 hrs)**

3.1 Analytical procedures involved in environmental monitoring. Water quality– BOD, COD, DO, nitrite, nitrate, iron, fluoride.

3.2 Soil- moisture, salinity, colloids, cation and anion exchange capacity.

3.3 Air pollution monitoring sampling, collection of air pollutants-SO_2, NO_2, NH_3, O_3 and SPM.

3.4 Analysis of metals, alloys and minerals. Analysis of brass and steel. Analysis of limestone. Corrosion analysis.

Unit 4: **Capillary Electrophoresis and Capillary Electro-chromatography** **(9 Hrs)**

4.1 Capillary electrophoresis–migration rates and plate heights, instrumentation, sample introduction, detection(indirect)-fluorescence, absorbance, electrochemical, mass spectrometric, applications. Capillary gel electrophoresis. Capillary isotachophoresis. Isoelectric focusing.

4.2 Capillary electro chromatography–packed columns. Micellar electro kinetic chromatography.

Unit 5: Process instrumentation **(9 Hrs)**

5.1 Automatic and automated systems, flow injection systems, special requirements of process instruments, sampling problems, typical examples of C, H and N analysers.

Unit 6: Aquatic Resources **(9 Hrs)**

6.1 Aquatic resources: renewable and non-renewable resources, estimation, primary productivity – factors affecting it, regional variations.

6.2 Desalination: principles and applications of desalination–distillation, solar evaporation, freezing, electrodialysis, reverse osmosis, ion-exchange and hydrate formation methods. Relative advantages and limitations. Scale formation and its prevention in distillation process.

6.3 Non-renewable resources: inorganic chemicals from the sea – extraction and recovery of chemicals, salt from solar evaporation.

References

01. J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.

02. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Publ., 2007.

03. R.D. Brownn, Introduction to Instrumental Analysis, McGraw-Hill, 1958.

04. H.H. Willard, L.L. Merritt, J.A. Dean, Instrumental Methods of Analysis, Van Nostrand, 1974.

05. G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.

06. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College, 1990.

07. J.G. Dick, Analytical Chemistry, R.E. Krieger, 1978.

08. E.D. Howe, Fundamentals of Water Desalination, Marcel Dekker, 1974.

09. H.G. Heitmann, Saline Water Processing, VCH, 1990.

SEMESTERS 3 and 4

PH4P04 PHARMACEUTICAL ANALYSIS PRACTICAL

Credit : 3 **Contact Lab Hours: 54+54=108**

1. Preparation, assay including limit tests prescribed in the IP/BP of the following drugs: sodium salicylate, calcium lactate, yellow mercuric oxide, ferrous fumarate, ferric ammonium citrate, potassium antimony citrate, boric acid, light magnesium carbonate, and sodium citrate.
2. Assay, test for identity and purity of the following synthetic drugs: aspirin, paracetamol, analgin, sulphadiazine (or any other sulphonamide), isoniazide, benzyl benzoate, piperazine, chloropromazine hydrochloride, diethyl carbamazine citrate, oxyphenbutazone, phenytoin sodium, ibuprofen, hexamine, tolbutamide and gamma benzene hexachloride.
3. Analysis of official drugs using common analytical techniques.
4. Assay of Antibiotics. Chemical Assay of Benzyl Pencillin
5. Assay of Vitamins: ascorbic acid, acetomenaphthone, niacinamide, pyridoxine and thiamine.
6. Assay of some alkaloids official in IP/BP: atropine, codeine, ephedrine and quinine. Ananlysis of liquid extracts of some alkaloidal content.
7. Evaluation of medicinal oils: eucalyptus oil, clove oil and camphor oil.

References

01. A.O. Bentley, J.E. Driver, Bentley and Driver's Textbook of Pharmaceutical Chemistry, 7th Edn., Oxford University Press, 1960.
02. G.L. Genkins, A.M. Knevel, F.E. DiGangi, Quantitative Pharmaceutical Chemistry, 7th Edn., McGraw Hill, 1977.
03. K.A. Connors, A Textbook of Pharmaceutical Analysis, John Wiley & Sons, 2007.
04. Indian Ministry of Health and Family Welfare, Indian Pharmacopoeia 1996, Controller of Publication, 2000.
05. British Pharmacopoeia Commission, British Pharmacopoeia:2012 Edition, Bernan Assoc, 2011

PH4P05 DRUG SYNTHESIS AND DISPENSING PRACTICAL

Credit : 3 **Contact Lab Hours: 54+54=108**

1. Synthesis of some typical organic medicinal compounds, spectral illustration of the intermediates and products formed:

   paracetamol, sulphanilamide, hippuran, benzocaine, clofibrate, mercurochrome, phenytoin, dapsone, diodoquin, antipyrine, aminacrine and phenobarbitone.

2. Preparation of some specified crude plant extracts and qualitative analysis (chemical or TLC) of crude plant extracts/ products to detect the presence of phytochemicals-alkaloids, carbohydrates, glycosides, tannins, flavanols and saponins.

3. Isolation of phytochemicals from their natural sources.

   Examples

   Caffeine from Tea
   Nicotine from tobacco
   Cucumin from turmeric
   Tannins from Gallnuts
   Lycopene from tomato

4. Dispensing

   01. Emulsions
      a. Castor oil emulsion
      b. Shark liver oil emulsion
      c. Liquid paraffin emulsion

   02. Liniments
      a. Turpentine liniment
      b. Methyl salicylate liniment
      c. Camphor liniment

   03. Ointments
      a. Compound benzoic acid ointment
      b. Non-staining iodine ointment

   04. Pastes
      a. Unnas paste
      b. Magnesium sulphate paste

05. Creams
    a. Vanishing cream
    b. Cetrimide cream

06. Paints
    a. Mandel's paint
    b. Tannic acid glycerine paint

07. Lotions
    Calamine lotion

08. Dentrifices
    a. Tooth paste
    b. Tooth powder

09. Mixtures
    Typical mixtures involving incompatibilities.

10. Tablets
    a. Aspirin tablet
    b. A P C tablets

References

01. T. E. Wallis, Practical Pharmacognosy, Churchill, 1948.
02. A.O. Bentley, J.E. Driver, Bentley and Driver's Textbook of Pharmaceutical Chemistry, 7th Edn., Oxford University Press, 1960.
03. K.A. Connors, A Textbook of Pharmaceutical Analysis, John Wiley & Sons, 2007.
04. J.W. Cooper, C. Gunn, Cooper and Gunn's Dispensing for Pharmaceutical Students, Pitman Medical, 1967.
05. A. Kar, Advanced Practical Medicinal Chemistry, New Age International, 2007.

PH4P06 BIOCHEMISTRY AND BACTERIOLOGY PRACTICAL

Credit : 3 **Contact Lab Hours: 72+72 =144**

A. Biochemistry

01. Blood Analysis
    a. Determination of blood group and Rh factor.
    b. Enumeration of RBC, WBC and differential leucocyte count.
    c. Determination of ESR.
    d. Estimation of urea, uric acid, cholesterol, creatinine, haemoglobin and calcium.
02. Urine Analysis
    a. Qualitative analysis of urine for the common pathological constituents-sugar, albumin, ketone bodies, bile.
    b. Estimation of albumin, ketone bodies, sugar and urea.
03. Milk Analysis

    Estimation of specific gravity, total solids, fat, lactose, total nitrogen, calculation of percentage of added water.
04. Water Ananlysis

    Estimation of total dissolved matter, chloride, saline and albuminoid ammonia and COD.
05. Preparation of some compounds of biochemical interest.

    Examples: caffeine, albumin, glutamic acid, urease, cholesterol, tyrosine.
06. Separation of amino acids by paper chromatography.
07. Separation of serum proteins by paper electrophoresis.

B. Bacteriology

01. Preparation of some typical nutrient media for collection and isolation of bacteria.
    a. Nutrient Agar, Endo's Agar, Chapman's Agar, Tergotol-7 Agar and McConkey Agar.
02. Staining and the study of the morphology of the bacteria.
    a. Simple stain
    b. Gram stain (Huker method)

c. Capsule stain
d. Acid fast stain (Ziehl- Neelson)
e. Negative stain (India ink method)

03. Fermentation test
04. Identification of some common pathogenic organisms.
05. Enumeration of bacteria in water.
06. Enumeration of bacteria in milk-the reductase test.
07. Evaluation of germicides-Riedel Walker test.
08. Antibiotic sensitivity tests.
09. Preparation and standardization of vaccines.
10. Preparation of lactic acid by fermentation of sugar.
11. Method of study of antibacterial activity of compounds and complexes.

References

01 A.J. Salle, Laboratory Manual of Fundamental Principles of Bacteriology, McGraw Hill, 1973.

02 R.C. Goss, Experimental Microbiology Laboratory Guide, Iowa State Univ. Press, 1967.

03 T.J. Mackie, J.E. McCartney, Handbook of Practical Bacteriology, E&S Livingstone, 1948.

04 P.B. Hawk, Hawk's Physiological Chemistry, Blakiston Division, 1965.

05 K. Wilson and J.M. Walker, Principles and Techniques of Practical Biochemistry, 5th Edn., Cambridge University Press, 2000.

06 M.B. Jacob, The Chemical Analysis of Food and Food products, Van Nostrand, 1958.

07 J.A. Kolmer, E.H. Spaulding, H.W. Robinson, Approved Laboratory Techniques, Appleton Century Crofts, 1951.

08 D.T. Pulmmer, An Introduction to Practical Biochemistry, McGraw Hill, 1987.