B. Sc. (HONS.) CHEMISTRY

<u>DISTRIBUTION OF DIFFERENT COURSES AND CREDITS IN VARIOUS SEMESTERS</u>

Offered By:

Department of Chemistry
Faculty of Science
Banaras Hindu University

Semester-wise Distribution of Courses and Credits

CHB-101: Section A - Structure and Bonding Section B - Organic Chemistry - I Section B - Organic Section B - Inorganic Chemistry - I Section B - Physical Chemistry - I Section B - Organic Chemistry - I Section B - Physical Chemistry - I Section B - Section B - Organic Chemistry - I Section B - Section B - Organic Chemistry - I Section B - Sec	Paper	Credits	Total Credits	
Section B - Organic Chemistry - I	<u>Semester-I</u>			
Section A: Quantitative Analysis (Physical & Volumetric) Section B: Qualitative Analysis (Organic & Inorganic) Semester-II		4		
Section B: Qualitative Analysis (Organic & Inorganic) Semester-II	CHB-102: Chemistry Practical-I			
CHB-201: Section A - Inorganic Chemistry-I Section B - Physical Chemistry-I Section B - Physical Chemistry-I Section B - Physical Chemistry-I Section B - Opaphic Chemistry-I Section B - Opaphic Chemistry-II Section B - Physical Chemistry-II Section B - Opaphic Chemistry-II Section B - Selected topics in Chemistry-II Section B - Selected topics in Chemistry II Section (A): Quantitative Analysis (Physical & Volumetric) Section (B): Preparations (Organic & Inorganic) 3* CHB-302: Chemistry Practical-IV Section (B): Preparations (Organic & Inorganic) 2 Semister-V CHB-402: Chemistry Practical-IV Section (B): Preparations (Organic & Inorganic) 2 Semister-V CHB-501: Analytical Chemistry-II 3 CHB-502: Inorganic Chemistry-III 3 CHB-503: Organic Chemistry-III 3 CHB-505: Inorganic Chemistry Practical 2 CHB-506: Organic Chemistry Practical 2 CHB-507: Physical Chemistry-IV 3 CHB-603: Organic Chemistry-IV 3 CHB-604: Physical Chemistry-IV 3 CHB-605: Inorganic Chemistry-IV 3 CHB-604: Physical Chemistry-IV 3 CHB-604: Physical Chemistry-IV 3 CHB-605: Inorganic Chemistry-IV 3 CHB-607: Physical Chemistry Practical 2 CHB-607: Physical Chemistry Practical 3 CHB-607: Phys		2	6	
Section B - Physical Chemistry-I	<u>Semester-II</u>			
Section A: Quantitative Analysis (Physical & Volumetric) 2		4		
Section B. Qualitative Analysis (Inorganic) Semester-III	CHB-202: Chemistry Practical-II			
CHB-301: Section A - Organic Chemistry-II Section B - Physical Chemistry-II Section (A): Quantitative Analysis (Physical & Volumetrie) Section (A): Quantitative Analysis (Physical & Volumetrie) Section (B): Qualitative Organic Analysis		2	6	
Section B - Physical Chemistry-II	Semester-III			
CHB-03A: Basic Aspects of Chemistry (for PMS & SMK groups only) 3* CHB-302: Chemistry Practical-III Section (A): Quantitative Analysis (Physical & Volumetric) 2 6 Semester-IV CHB-401: Section A - Inorganic Chemistry-II Section B - Selected topics in Chemistry 4 4 CHB-401: Section A - Inorganic Chemistry (for PMK group) 3* CHB-302: Chemistry Practical-IV Section (A): Quantitative Analysis (Physical & Volumetric) Section (B): Preparations (Organic & Inorganic) 2 6 Semester-V CHB-501: Analytical Chemistry-II 3 3 CHB-502: Inorganic Chemistry-III 3 CHB-503: Organic Chemistry-III 3 CHB-504: Physical Chemistry Practical 2 CHB-505: Inorganic Chemistry Practical 2 CHB-506: Organic Chemistry Practical 2 CHB-601: Analytical Chemistry-IV CHB-602: Inorganic Chemistry-IV CHB-603: Organic Chemistry-IV 3 CHB-605: Inorganic Chemistry-IV 3 CHB-606: Organic Chemistry Practical CHB-607: Ph		4		
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CHB-401: Section A - Inorganic Chemistry-II Section B - Selected topics in Chemistry	Section (A): Quantitative Analysis (Physical & Volumetric)	2	6	
Section B - Selected topics in Chemistry			r	
CHB-402: Chemistry Practical-IV Section (A): Quantitative Analysis (Physical & Volumetric) Section (B): Preparations (Organic & Inorganic) 2		4		
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CHB-606: Organic Chemistry Practical 2 CHB-607: Physical Chemistry Practical 2 CHB-608: Elective Paper - Section-A: Atomic and Molecular Structure	CHB-604: Physical Chemistry-IV	3		
CHB-607: Physical Chemistry Practical CHB-608: Elective Paper - Section-A: Atomic and Molecular Structure	CHB-605: Inorganic Chemistry Practical	2		
CHB-608: Elective Paper - Section-A: Atomic and Molecular Structure	CHB-606: Organic Chemistry Practical	2		
Section D. Application of Section 2017.	CHB-607: Physical Chemistry Practical	2		
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Total 64	*			

Semester- I

CHB-101

Credits: 4

Section (A): Structure and Bonding

- 1 **Atomic Structure:** Schrodinger wave equation; H atom; Radial and angular wave functions: quantum numbers and concept of orbitals; Slater orbitals.
- 2 **Chemical Bonding**: VB and MO approach of H₂ molecule; MO treatment of homonuclear and heteronuclear (CO & NO) diatomic molecules; Concept of HOMO and LUMO. VSEPR theory; Structure of simple molecules and ions of main group elements
- 3 **Ionic Solids:** Close packing, Radius ratio rule and crystal coordination number. Examples of MX and MX2 type ionic solids (NaCl and TiO₂)
- 4 Metallic Bonding: theories of bonding in metals; Free electron, VB and Band theories.
- 5 Weak Interactions: Hydrogen bonding and van der Waal's interactions

Section (B): Organic Chemistry-I

- 1 **Concepts:** Atomic orbitals, hybridization, orbital representation of methane, ethane, ethyne and benzene. Polarity of bonds: Inductive, resonance and steric effects hyperconjugation, and their influence on acidity and basicity of organic compounds.
- 2 **Hydrocarbons:** Akanes: Chlorination of methane, Alkenes: Addition reactions (Electrophilic and Free radical), Hydration, hydroxylation, hydroboration, epoxidation and ozonolysis. Alkynes: Reduction, Electrophilic addition, acidity and metal acetylides. Conjugated and isolated Dienes: 1,2- verses 1,4-addition. Diels Alder reaction.
- 3 **Alkyl Halides:** Nucleophilic substitution: SN¹, SN² mechanisms; Eliminations reactions: E1and E 2 mechanisms, Elimination versus substitution reactions; energy profile diagrams-transition states (general considerations). Grignard reagents: Preparation and synthetic applications.
- 4 **Alcohols:** Comparative study of substitution, dehydration, oxidation, and esterification of primary, secondary and tertiary alcohols.
- 5 **Stereochemistry:** Fischer, Saw-horse and Newman projection formulae, Chirality-optical activity, enantiomersim and diasteroisomerism involving one and two chiral centres. Configuration; D/L, erythrose, threose and R/S nomenclatures. Geometrical isomerism and E/Z nomenclatures. Conformations of n-butane.
- 6 *Active methylene compounds:* Preparation and synthetic applications of ethyl acetoacetate and diethyl malonate, Tautomerism.

Books Recommended

For Section-A

- 1. Basic Inorganic Chemistry, F. A Cotton, G. Wilkinson, and Paul L. Gaus, 3rd Edition (1995), John Wiley & Sons, New York.
- 2. Concise Inorganic Chemistry, J. D. Lee, 5th Edition (1996), Chapman & Hall, London.

For Section-B

- 1. Organic Chemistry, Paula Y. Bruice, 2nd Edition, Prentice-Hall, International Edition (1998).
- 2. Organic Chemistry, I. L. Finar, Vol. I, 6th Edition (1973), ELBS and Longman Ltd., New Delhi.
- 3. Organic Chemistry, R. T. Morrison and R. N. Boyd, 6th Edition (1992), Prentice-Hall of India (P) Ltd., New Delhi.
- 4. Organic Chemistry, Paula Y. Bruice, 2nd Edition, Prentice-Hall, International Edition (1998).
- 5. Organic Chemistry, I. L. Finar, Vol. I, 6th Edition (1973), ELBS and Longman Ltd., New Delhi.
- 6. Organic Chemistry, R. T. Morrison and R. N. Boyd, 6th Edition (1992), Prentice-Hall of India (P) Ltd., New Delhi.
- 7. Organic Chemistry, J. Clayden, N. Greeves, S. Warren, and E. Wothers, Oxford Univ. Press, Oxford (2001).

CHB-102 Credits: 2

Section-A: Quantitative Analysis (Physical and Volumetric)

- 1. Kinetics of First Order reaction.
- 2. Redox titration: (a) Iodometry (b) Fe2⁺ / K₂Cr₂O₇

Section-B: Qualitative Analysis (Organic and Inorganic):

- 1. Detection of elements (X, N, S)
- 2. Detection of functional groups: PhOH, -COOH, C=O, -CHO, Ar-NH₂, Ar-NO₂, -CONH₂
- 3. Qualitative Inorganic Mixture Analysis: Anions and interfering anions.

Note: Experiments may be added/deleted subject to availability of time and facilities.

Semester- II

CHB-201

Credits: 4

Section (A) - Inorganic Chemistry-I

- 1. **Periodic trends and properties**: Size, Ionization Energy, Electron Affinity, Electronegativity, Lattice and Hydration Energies, Use of redox potential and reaction feasibility
- 2. Chemistry of s and p-block elements: Alkali and alkaline earth metals: Hydrides and Complexation tendencies. Structural features of hydrides, halides, oxides and oxyacids
- 3. **Chemistry of** *d***-block elements**: Salient features, characteristic properties of 3*d*-elements with reference to oxidation states, colour, magnetic behaviour, and complex formation tendency.

Section (B) - Physical Chemistry-I

- 1. *Gaseous State*: Kinetic theory of gases, ideal gas laws based on kinetic theory. Collision in a gas- mean free path, collision diameter, collision number. Behaviour of real gases the van der Waal's equation. Critical phenomena critical constants of a gas and their determination, the van der Waals equation and critical state, Principle of corresponding states.
- 2. *Liquid State*: Surface tension of liquids capillary action, experimental determination of surface tension, temperature effect on surface tension. Viscosity of liquids, experimental determination of viscosity coefficient, its variation with temperature.
- 3. *Thermodynamics:* First Law of thermodynamics and internal energy, state and state functions, sign convention for heat and work, nature of work, path dependence of heat and work. Enthalpy, heat changes at constant volume and constant pressure, heat capacities (C_V, C_P) and their relationship for ideal gases.
 - Thermodynamic quantities $(w, q, \Delta U, \Delta H)$ for isothermal and adiabatic reversible expansion of ideal gases and their comparison.
 - Change in internal energy (ΔU) and enthalpy (ΔH) of chemical reactions, relation between ΔU and ΔH , variation of heat of reaction with temperature (Kirchhoff's equation).
- 4. *Electrochemistry*: Arrhenius theory of electrolytic dissociation, Hydrolysis of salts, hydrolysis constant, buffer solutions, indicators and theory of acid-base indicators.

 Migration of ions: transference number and its determination by Hittorf methods. Conductance of

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electrolyte solutions, molar conductance of electrolyte and its splitting into ionic molar conductance, Kohlrausch law of independent migration of ions, ionic mobility. Application of conductance measurements: determination of degree of dissociation and dissociation constant of weak electrolytes/acids, solubility of sparingly soluble salts, and Conductometric titrations.

5. *Nuclear Chemistry*: Nucleus and its classification, nuclear forces, nuclear binding energy, stability of nucleus. Radioactivity: Radioactive elements, general characteristics of radioactive decay, decay kinetics (decay constant, half life, mean life period), units of radioactivity.

Books Recommended

For Section-A

- 1. Basic Inorganic Chemistry, F. A Cotton, G. Wilkinson, and Paul L. Gaus, 3rd Edition (1995), John Wiley & Sons, New York.
- 2. Concise Inorganic Chemistry, J. D. Lee, 5th Edition (1996), Chapman & Hall, London.

For section-B

- 1. *Physical Chemistry*, P. Atkins and J. De Paul, 8th Edition (2006), International Student Edition, Oxford University Press.
- 2. *Physical Chemistry*, P. C. Rakshit, 5th Edition (1988), 4th Reprint (1997), Sarat Book House, Calcutta.
- 3. *Principles of Physical Chemistry*, B. R. Puri, L. R. Sharma, and M. S. Pathania, 37th Edition (1998), Shoban Lal Nagin Chand & Co., Jalandhar.
- 4. *Physical Chemistry*, K. J. Laidler and J. M. Meiser, 3rd Edition, Houghton Mifflin Comp., New York, International Edition (1999)

CHB-202 Credits: 2

Section-A: *Quantitative Analysis (Physical and Volumetric)*

- 1. Determination of water equivalent of a calorimeter (cooling curve).
- 1. Heat of neutralization (strong acid-strong base).
- 2. Heat of dissociation of weak acid.
- 3. Heat of solution (NH₄NO₃, CaCl₂).
- 4. Basicity of an acid by thermochemical method.

Section-B: Qualitative Inorganic Analysis

Qualitative Inorganic Mixture Analysis: Not containing more than 4 ions and one interfering anion

Note: Experiments may be added/deleted subject to availability of time and facilities.

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Semester- III

CHB-301

Credits: 4

Section (A):Organic Chemistry-II

- 1. **Aromaticity:** Aromaticity and Huckel rule A general concept. Molecular orbital picture of benzene.
- 2. **Aromatic Electrophilic Substitution:** Mechanism of nitration, halogenation, sulphonation, and Friedel-Crafts (alkylationa and acylation) reactions. Effects of substituents on orientation and reactivity.
- 3. **Aryl Halogen Compounds:** Chlorobenzene, electrophilic and nucleophilic aromatic substitutions; side chain chlorination of toluene, DDT and BHC.
- 4. **Chemistry of Carbonyl compounds:** Preparations and reactions: addition and condensation reactions; Cannizzaro, Perkin, aldol, benzoin, haloform, oxidation and reduction reactions. Important reactions of acids, HVZ reaction, Relative reactivity of acid chlorides, acid anhydrides, amides and esters. Comparative acidity of carboxylic and sulphonic acids.
- 6. **Phenols:** General methods of preparation and reactions. Reimer-Tiemann and Kolbe reactions. Relative acidity of phenol, alcohol and carboxylic acid.
- 7. **Nitrogen Containing compounds:** Nitronbenzene and reduction products. Comparative basicity of aliphatic and aromatic amines. **Diazonium Salts**: Preparation and synthetic applications.

Section (B): Physical Chemistry-II

1. *Thermodynamics:* Second Law of Thermodynamics, Carnot cycle, entropy, entropy changes in reversible and irreversible processes and of universe, physical concept of entropy, entropy changes of an ideal gas in different processes, entropy of an ideal gas, entropy changes in mixture of gases. Joule-Thomson effect, Joule-Thomson coefficient of real (van der Waal) gases, inversion temperature.

Free energy and its concept, Gibbs and Helmholtz free energies and their relationship, variation of free energy with temperature and pressure. Free energy and equilibrium constant. Maxwell's relations, Gibbs-Helmholtz equations, its application for the determination of ΔG , ΔH , ΔS of a reversible cell reaction. Criteria for reversible and irreversible processes based on entropy and free energy.

Partial molal quantities, chemical potential, the Gibbs-Duhem equation, determination of partial molal quantities, variation of chemical potential with temperature and pressure, chemical potential in case of a system of ideal gases.

- 2. *Phase Equilibria*: Thermodynamics of phase transition-Clapeyron-Clausius equation and its applications. Phase rule, phase, component, degree of freedom, thermodynamic derivation of phase rule, phase diagrams of one-component system (water), two component systems (phenolwater, lead-silver). The distribution law, applications to cases of dissociation and association of solutes in one of the phases, solvent extraction, equilibrium constant from distribution coefficient (KI + I₂ = KI₃).
- 3. *Electrochemical Cells*: Reactions in reversible cells, free energy and *emf* of reversible cell. Single electrode potential (Nernst equation), its measurement and sign convention. Standard electrode potential. *Emf* of reversible cell from electrode potentials. Types of reversible

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- electrode, reference electrodes. Applications of emf measurements: determination of ionic activities, pH, and equilibrium constant. Potentiometric titration. Concentration cells with and without transference. Liquid junction potential and its elimination.
- 4. *Chemical Kinetics*: Order and molecularity of chemical reactions, pseudo order. Kinetic law for second order reactions, determination of the rate constant and order of reaction from kinetic data. Effect of temperature on rate of reaction: collision theory of rates of bimolecular reactions and its comparison with Arrheninus equation.

Complex reactions: Reversible (first order in both directions), concurrent, consecutive reactions. Unimolecular gas reactions (Lindmann theory), steady-state approximations, theory of absolute reaction rate and its thermodynamic formulation.

Books Recommended

For Section-A

- 1. Organic Chemistry, Paula Y. Bruice, 2nd Edition, Prentice-Hall, International Edition (1998)
- 2. Organic Chemistry", R. T. Morrison and R. N. Boyd, 6th Edition (1992), Prentice-Hall of India (P) Ltd., New Delhi.
- 3. Organic Chemistry, I. L. Finar, [Vol. I, 6th Edition (1973), Reprinted in 1980 & Vol. II, 5th Edition (1975), Reprinted in 1996], ELBS and Longman Ltd., New Delhi.
- 4. Organic Chemistry, L.G. Wade Jr., 5th Edition (2001) Prentie Hall International INC, USA.
- 5. Organic Chemistry, J. Clayden, N. Greeves, S. Warren, and E. Wothers, Oxford Univ. Press, Oxford (2001).

For Section-B

- 1. Physical Chemistry, P. C. Rakshit, 5th Edition (1985), 4th Reprint (1997), Sarat Book House, Calcutta
- 2. Principles of Physical Chemistry, B. R. Puri, L. R. Sharma, and M. S. Pathania, 37th Edition (1998), Shoban Lal Nagin Chand & Co., Jalandhar.
- 3. *Physical Chemistry*, K. J. Laidler and J. M. Meiser, 3rd Edition, Houghton Mifflin Comp., New York, International Edition (1999).

CHB-302 Credits: 2

Section-A: *Quantitative Analysis (Physical and Volumetric)*

- 1. Critical Solution Temperature.
- 2. Effect of impurity on Critical Solution Temperature.
- 3. Distribution of solute in two immiscible solvents (without association).
- 4. Distribution of solute in two immiscible solvents (with association in one solvent).
- 5. Determination of pH of a given buffer.

Section-B: *Qualitative Organic Analysis*

Identification of simple organic compounds (derivatives not included)

Note: Experiments may be added/deleted subject to availability of time and facilities.

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Semester IV

CHB-401

Credits: 4

Section (A): Inorganic Chemistry-II

- 1. **Acids and bases**: Bronsted-Lowry, Lux-Flood, Solvent System and Lewis concepts of acids and bases. Factors affecting strengths of Lewis acids and bases. HSAB theory and applications
- 2. **Non-aqueous solvents:** Physical properties of a solvent for functioning as an effective reaction medium, types of solvents and their general characteristics. Liq. NH₃ as a non-queous solvent
- 3. **Coordination compounds:** Nomenclature, Werner's theory. Isomerism. Sidgwick's EAN concept and Valence Bond Theory. Stereochemistry of coordination compounds with coordination no. 4, 5 and 6.
- 4. **Lanthanides:** Comparative study of lanthanide elements with respect to electronic configuration atomic and ionic radii, oxidation state and complex formation, lanthanide contraction. Separation of lanthanides. Application of lanthanide complexes.

Section (B): Selected Topics in Chemistry

- 1. **Energy devices:** Batteries; Fuel cells, Solar cells, Biomass as renewable energy resources.
- 2. **Corrosion:** Causes of metallic corrosion, types of corrosion, measurements of corrosion by weight loss method, prevention (electrochemical and inhibitor).
- 3. **Green Chemistry:** Principles and concept of green chemistry, atom economic and non-economic reactions, reducing toxicity, a few examples of environmental friendly reactions and reaction media
- 4. **Photoisomerization:** Rotation about C-C and C=C bonds, Structure of Rhodospin, Mechanism of vision.
- 5. **Bioenergetics:** Gibbs and Helmholtz energies with special emphasis on biological applications: study of energy transformations in living systems (bioenergetics): standard state in biochemistry, ATP-the currency of energy, Glycolysis, limitation of applicability of thermodynamics in biology.

Books RecommendedFor Section-A

- 1. Recent Aspects in Inorganic Chemistry, R.C. Agarwal, Kitab Mahal
- 2. *Inorganic Chemistry*, J.E. Huheey, E.A. Keiter and R.L. Keiter.
- **3.** *Basic Inorganic Chemistry*, F. A Cotton, G. Wilkinson, and Paul L. Gaus, 3rd Edition (1995), John Wiley & Sons, New York.

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For Section-B

- 1. Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang; University Science Book, California (2000).
- 2. New Trends in Green Chemistry, V.K. Ahluwalia, M. Kidwai, Anamaya Publication, New Delhi (2004)
- 3. Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang; University Science Book, California (2000).
- 4. New Trends in Green Chemistry, V.K. Ahluwalia, M. Kidwai, Anamaya Publication, New Delhi (2004)
- 5. Green Chemistry: Environmentally Benign Reactions, V. K. Ahluwalia, 2007
- 6. *Modern Molecular Photochemistry*, N. J. Turro, University Science Books, Sausalito California (1991).
- 7. Green Chemistry: An Introductory Text, Mike Lancester, RSC Paperback, Edn. (2002)

CHB-402 Credits: 2

Section-A: *Quantitative Analysis (Physical and Volumetric)*

- 1. Coagulation of a sol.
- 2. Determination of Surface Tension of liquids.
- 3. Determination of viscosity coefficients of liquids.
- 4. Complexometric titrations: Zn²⁺, Mg²⁺, Ca²⁺, Fe²⁺ with EDTA; Hardness of water.
- 5. Iodimetric titration.

Section-B: *Preparations* (Organic and Inorganic)

- 1. Preparation of Organic Compounds:
 - (i) m-dinitrobenzene, (ii) Acetanilide, (iii) Bromoacetanilide, (iv) Oxidation of primary alcohols-Benzoic acid from benzylacohol, (v) azo dye
- 2. Preparation of Inorganic Compounds:
 - (i) Potassium trioxalato chromate (III); (ii) CoHg(SCN)₄; (iii) Cu(I) thiourea complex
 - (iv) Bis (2, 4-pentanedionate) zinc hydrate; (v) Double salts (Chrome alum/ Mohr's salt)

Note: Experiments may be added/deleted subject to availability of time and facilities.

Semester V

CHB-501: Analytical Chemistry-I

Credits: 3

- 1. **Stastical Evaluation:** Determinant and indeterminant errors, Normal error curve, Accuracy and Precision, Relative and standard deviation, Methods for minimizing errors, Criteria for rejection of observation, Significant figures and computation rules, Error propagation.
- 2. **Precipitation:** Desirable properties of gravimetric precipitates, Formation of gravimetric precipitates, Conditions for quantitative precipitations, Contamination in precipitates, Method for removal of impurities in precipitates, Steps involved in quantitative

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- precipitation, Organic precipitants (oxine, dithizone, α -nitroso-(naphthol, cupferon, dimethyl glyoxime) in chemical analysis.
- 3. **Analytical Reagents:** Theoretical and practical aspects of the use of EDTA, cerate, iodate, bromate, chloramine-T, Karl Fischer and periodate reagents in chemical analysis.
- 4. **Environmental Pollution:** Terminology used in environmental chemistry, Atmospheric pollution, Source of air pollution, Global warming, Ozone-hole, Auto exhaust emissions and it's prevention, Air quality parameters, Acid rains, Industrial and domestic effluents, Treatment plants, Flouresis, Arsenic, Mercury and Methylisocynate(MIC) poisonings, Current environmental issues in the national context and remedial measures.

Books Recommended:

- 1. 'Modern Methods of Chemical Analysis', R.L. Pecscock, L.D. Shields, T. Cairns, and I.C. Mc William, 2nd Edition (197 6), John Willey, New York.
- 2. 'Basic Concepts of Analytical Chemistry', S.M.Khopkar, 2nd edition (1998), New Age International Publications, New Delhi.
- 3. 'Analytical Chemistry', G.D. Christian, John Willey & sons, New York (200 1)
- 4. 'Environmental Chemistry', A.K. De, 3rd edition (1994), Willey Eastern, New Delhi.

CHB-502: Inorganic Chemistry-III

Credits: 3

- 1. *Theories of Metal-Ligand bonding:* Limitations of valence bond theory; Crystal-field theory and crystal-field splitting in octahedral, tetrahedral and square planar complexes. Jahn-Teller Distortion. Factors affecting the crystal-field splitting.
- 2. *Thermodynamic and Kinetic aspects of Metal Complexes:* A brief outline of thermodynamic and kinetic stabilities of metal complexes and factors affecting the stability. Substitution reactions of square-planar complexes Trans effect
- 3. *Chemistry of Second and Third Transition Series:* A general comparative treatment of 4d and 5d elements with their 3d analogues in respect of ionic radii, oxidation states, magnetic behaviour and electronic spectral properties
- 4. *Organometallic Chemistry:* Definition, nomenclature and classification of organometallic compounds. Preparation, properties, bonding and applications of alkyl and aryls of Li, Al, Hg, Sn, Ti. A brief account of metal-ethylenic complexes and homogeneous hydrogenation

Books Recommended

- 1. "Concise Inorganic Chemistry", J. D. Lee, 5th Edition (1996), Chapman & Hall, London.
- 2. "Inorganic Chemistry", J.E. Huheey, E.A. Keiter and R.L. Keiter.
- 3. "Modern Inorganic Chemistry", R. C. Aggarwal, 1st Edition (1987), Kitab Mahal, Allahabad.
- 4. "Basic Inorganic Chemistry", F. A Cotton, G. Wilkinson, and Paul L. Gaus, 3rd Edition (1995), John Wiley & Sons, New York.
- 5. "Inorganic Chemistry", A. G. Sharpe, 3rd International Student Edition (1999), ELBS / Longman, U.K.
- 6. "Inorganic Chemistry", D. F. Shriver and P. W. Atkins, 3rd Edition (1999), ELBS, London.

- 1. **Alicyclic Compounds:** Cycloalkanes, general synthesis, Bayer's strain Theory. Cyclohexane-chair and boat conformations, axial and equatorial bonds, conformation of mono substituted cyclohexanes.
- 2. **Poly nuclear Hydrocarbons:** Alternant and non-alternant hydrocarbons. Chemistry of naphthalene.
- 3. Reactive intermediates and related Rearrangement reactions: Generation, stability and reactivity of *Free radicals* (Anti Markovnikov's, Birch Reduction, Bouveault-Blanc reduction, oxidation of phenol by metal ions); *Carbocations* (Pinacol-Pinacolone, Wagner-Meerwein Rearrangement, Baeyer-Villiger oxidation, Hydroperoxide reaction and Beckmann.) and *Carbanions* (Robinson Annulation and Michael Addition); *Carbenes* and *Nitrenes* (Hofmann, Curtius reactions). Ylides: Sulphur ylides, phosphorous ylides, Michaelis-Arbuzov phosphonate synthesis, Witting reactions, Mitsunobu reaction.
- 4. **Isotope Effect in a Reaction:** Isotopic substitution in a molecule, primary and secondary kinetic isotope effects, solvent isotopic effect and their importance in mechanistic studies.
- 5. **Stereochemistry:** Concept of Chirality; symmetry element, symmetry operations. Enantiomers, diastereomers, racemates, racemisation, resolution, Pro-chirality, pro-stereoisomerism with suitable examples of one and two chiral centers. Regioselective, chemoselective and stereoselective reactions. Asymmetric induction, Cram's Rule: Addition of nucleophile to carbonyl function; Aldol condensation (*achiral-achiral*). Wilkinson's hydrogenation.
- 6. **Photochemistry:** Principles of photochemistry, photochemical reactions of carbonyl compounds and olefins.
- 7. **Heterocyclic Compounds:** Synthesis and chemistry of furan, pyrrole, pyridine, Indole and Ouinoline

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8. Books Recommended

- 1. Organic Chemistry, I. L. Finar, Vol. <u>I and II</u>, 5th Edition (1975), Reprinted in1996, ELBS and Longman Ltd., New Delhi.
- 2. Stereochemistry of Organic Compounds, **D. Nasipuri**, 2nd Edition (1994), Wiley Eastern Ltd., New Delhi
- 3. Stereochemistry of Organic Compounds, E.L. Eliel, S.H. Wilen and Mander, , Wiley Interscience, New York (2004).
- 4. Organic Chemistry, J. Clayden, N. Greeves, S. Warren, and E. Wothers, Oxford Univ. Press, Oxford (2001).
- 5. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, 6th Edition (1997), Orient Longman Ltd., New Delhi.
- 6. Organic Chemistry, R.T. Morrison and R.N. Boyd, 6th Edition (2003), Prentice- Hall of India, New Delhi.
- 7. Heterocyclic Chemistry: Syntheses, Reactions and Mechanisms, R.K. Bansal, 3rd Edition (1999), New Age International, Publisher, New Delhi.
- 8. Photochemistry and Pericyclic Reactions, Jagdamba Singh and Jaya Singh 2nd edition. New Age International (P) Ltd. Publishers, New Delhi

- 1. Solid State: Crystal lattices, space lattice, unit cell, crystal systems, law of rational indices, Miller indices, crystals and x-rays (the Braggs equation). Crystal structure of NaCl, graphite, and diamond. Types of crystal (molecular, covalent, metallic, ionic). Imperfection in crystals: point defect-Schottky and Frankel defects.
- 2. Surface and Photochemistry: Gibbs Adsorption isotherm. Multi layer adsorption-BET equation (no derivation) and its application to surface area measurement. Heterogeneous catalysis (surface reactions): kinetics of unimolecular surface reactions- inhibition and activation energy. Nature of surface. Kinetics of enzymatic reactions: Michaelis-Menten equation, effect of temperature and pH.
 - Law of photochemical equivalence, quantum efficiency, reasons for low and high quantum efficiency. Kinetics of photochemical reaction (H2+Br2=HBr), photostationary state, Chemical actinometers (uranyl oxalate)
- 3. Thermodynamics of Solutions: Chemical potential of a mixure of ideal gases. Chemical potential of real gases and fugacity, activity and activity coefficient (concept and physical significance), reference and standard states. Variation of fugacity with temperature and pressure, Lewis-Randall rule, thermodynamic functions of mixing (ΔG_{mix}, ΔS_{mix}, ΔV_{mix}, ΔH_{mix}), ideal solutions and their characteristic properties, Duhem-Margules equation and its application, Henry and Raoult's laws. Thermodynamics of colligative properties: Freezing point depression, elevation of boiling point, osmotic pressure. van't Hoff equation. Measurement of osmotic pressure and determination of molecular weight of macromolecules.
- 4. Electrochemistry: Theory of strong electrolytes: Qualitative idea of Debye-Huckel theory of ion-ion interactions, Debye-Huckel limiting law for activity coefficient of ions in electrolyte solution (derivation not required), its modification for concentrated solutions. Debye-Huckel-Onsager (D-H-O) theory of electrolytic conductance: qualitative idea of electrophoretic and relaxation effects, D-H-O equation for conductance of electrolyte solutions, effect of high frequency and high field on conductance.
- 5. Nuclear and Radiation Chemistry: Nuclear reactions: Bethe notation, types of nuclear reactions (n, p, α , d and γ), conservation of quantities (mass-energy and linear momentum) in nuclear reactions, reaction cross-section, compound nucleus theory and nuclear reactions. Nuclear fission: the process, fragments, mass distribution, and fission energy. Nuclear reactor: the natural uranium reactor, classification of reactors, breeder reactor. Nuclear fusion and stellar energy.
 - Radiation chemistry: Elementary ideas of radiation chemistry, radiolysis of water and aqueous solutions, unit of radiation chemical yield (G-value), radiation dosimetry (Fricke's dosimeter), units of radiation energy (Rad, Gray, Rontgen, RBE, Rcm, Sievert).

Books Recommended

- 1. *Physical Chemistry*, P. C. Rakshit, 5th Edition (1988), 4th Reprint (1997), Sarat Book House, Calcutta.
- 2. *Physical Chemistry*, K. J. Laidler and J. M. Meiser, 3rd Edition (International Edition, 1999), Houghton Mifflin Co., New York.
- 3. *Physical Chemistry*, I. N. Levine, 4th Edition (International Edition, 1995), Mc Graw-Hill Inc., New York.
- 4. Essentials of Nuclear Chemistry H. J. Arnikar, 4th Edition (1995), New Age International (p) Ltd., Wiley Eastern Ltd., New Delhi.

CHB-505: Inorganic Chemistry Practical

- 1. Chromatographic separation of metal ions.
- 2. Gravimetric estimation of Cations/Anions.

CHB-506: Organic Chemistry Practical

1. Systematic identification of organic compounds (monofunctional and bi-functional) and preparation of their derivatives.

Credits: 2

Credits: 2

Credits: 2

Credits: 3

CHB-507: Physical Chemistry Practical

- 1. Viscosity-composition curve for a binary liquid mixture.
- 2. Surface tension-composition curve for a binary liquid mixture.
- 3. Determination of indicator constant colorimetry.
- 4. Determination of pH of a given solution using glass electrode.
- 5. Beer's Law Determination of concentration of solution by colorimetry.
- 6. Order of reaction of I₂ / Acetone / H⁺.
- 7. Equilibrium constant of methyl acetate hydrolysis reaction

Note: Experiments may be added/deleted subject to availability of time and facilities.

Semester VI

CHB-601: Analytical Chemistry-II

- 1. **Solvent Extraction:** Distribution law, Single extraction, Multiple extraction, Craig concept of counter-current distribution, Important solvent systems: chelate extraction, synergic extraction, extraction by solvation, ion-pair extraction
- 2. **Chromatography:** Classification of chromatographic methods, General principle and application of adsorption, partition, ion exchange, thin layer, and paper chromatography.
- 3. Radio-Analytical Methods: Elementary theory, Isotope dilution and Neutron activation methods and applications.
- 4. **Spectrophotometry:** Beer's law and it's application, Nomenclature and units, General instrumentations for spectrophotometry, Spectrophotometric determinations of one Component (iron, chromoium, manganese, nickel, titanium and phosphorus) and two components (overlapping and non overlapping) systems, Spectrophotometric determination of dissociation constants of indicator, Photometric errors and RINGBOM-AYRES plots.

Book Recommended:

- 1. Principles of Instrumental Analysis, D.A. Skoog, F.J.Holler and T.A. Nieman, , 5th edition (1998), Horcourt Brace & Company, Florida.
- 2. Analytical Chemistry, G.D. Christian, John Willey & sons, New York (200 1).
- 3. Instrumental Methods of Analysis', H.H. Willard, L.L. Merritt, and J.A.Dean, 6th edition(1986), CBS Publishers & Distributors, Shahdara, Delhi.

4. Modem Methods of Chemical Analysis, R.L. Pecscock, L.D. Shields, T. Cairns, and I.C. Mc William, 2nd edition(1976), John Willey, New York.

CHB-602: Inorganic Chemistry-IV

1. *Magnetic Properties of Transition Metal Complexes*: Types of magnetic behaviour, methods of determining magnetic susceptibility, L-S and J-J coupling, orbital contribution to magnetic moments. Correlation of magnetic moment data and stereochemistry of Co(II) and Ni(II) complexes; anomalous magnetic moments.

Credits: 3

Credits: 3

- 2. *Electronic Spectra of Transition Metal Complexes*: Types of electronic transitions, selection rule for dd transitions, spectroscopic ground states. Explanation of electronic spectra on the basis of Orgel energy level diagrams for d1, d4, d6 and d9 states.
- 3. *Chemistry of f-block Elements*: Comparative study of actinide elements with respect to electronic configuration, atomic and ionic radii, oxidation states and complex formation; occurrence and principles of separation. General features and chemistry of actinides, principles of separation of Np, Pu and Am from U. Trans-Uranium elements.
- 4. **Bioinorganic Chemistry**: Essential and trace element in biological process, oxygen transport with reference to haemoglobin; synthetic models of O₂ carrieres., Biological role of alkali metals ions. Vitamin B-12

Books Recommended

- 1. Concise Inorganic Chemistry, J. D. Lee, 5th Edition (1996), Chapman & Hall, London.
- 2. Inorganic Chemistry, J.E. Huheey, E.A. Keiter and R.L. Keiter.
- 3. Modern Inorganic Chemistry, R. C. Aggarwal, 1st Edition (1987), Kitab Mahal, Allahabad.
- 4. Basic Inorganic Chemistry, F. A Cotton, G. Wilkinson, and Paul L. Gaus, 3rd Edition (1995), John Wiley & Sons, New York.
- 5. *Inorganic Chemistry*, A. G. Sharpe, 3rd International Student Edition (1999), ELBS / Longman, U.K.
- 6. Inorganic Chemistry, D. F. Shriver and P. W. Atkins, 3rd Edition (1999), ELBS, London

CHB-603: Organic Chemistry-IV

- 1. **Peptide Chemistry:** Amino acids-preparative methods, physical properties, dipolar nature, chemical reactions and configuration. *Peptides:* peptide linkage, peptide synthesis and structure of poly peptides. *Proteins:* General characteristics and secondary structure.
- 2. **Drugs:** Preparations, and uses of following: (i) Antipyretics and Analgesics: Aspirin, Paracetamol, Phenylbutazone. (ii) Sulpha Drugs: Sulphanilamide, sulphapyridine, sulphathiazole. (iii) *Antimalarials:* Chloroquine, Primaquine. (iv) *Antibiotics:* Chloroamphenicol.
- 3. **Carbohydrates:** Characteristic reactions of aldoses and ketoses. Glucose-structure (Open and Cyclic), Fructose (only reactions), Mutarotations, Sucrose, starch and cellulose (Structure<u>al</u> aspects only).

- 4. **Polymers:** Types of polymers and polymerization process: Addition, stereo controlled, step growth polymerizations. Radical, ionic and coordination mechanisms of polymerization. Synthesis and applications of following polymers: (i) Specialty Polymers: Conducting & Electroluminescent (Organic light emitting diodes), liquid crystals (ii) Natural and synthetic rubber (iii) Synthetic Fibers: Polyester, Polyamides (iv) Foaming Agent: Plasticizers (v) biodegradable polymers.
- 6. **Terpenes:** Occurrence, isolation, classification. Isoprene rule. Structure and synthesis of Citral and Geraniol.
- 7. **Dyes:** synthesis of malachite green, fluorescein. Synthesis and structure of Indigotin.

Books Recommended

- 1. Organic Chemistry, I. L. Finar, Vol. II, 5th Edition (1975) Reprinted in 1996, ELBS and Longman Ltd, New Delhi
- 2. Organic Polymer Chemistry, K. J. Saunders, 2nd Edition (1988), Chapman & Hall, London
- 3. Introduction to Synthetic Polymers, **Ian M. Campbell**, 2nd Edition (2000), Oxford University Press, USA
- 4. Principles of Polymer Science, P. Bahadur and N.V. Sastry, Narosa, New Delhi (2002).
- 5. *Principles of Medicinal Chemistry*, **W. O. Foye**, , 3rd Edition (1989), Lea & Febiger/ Varghese Publishing House, Bombay.
- 6. Medicinal Chemistry, A. Kar. Wiley Eastern Ltd., New Delhi (1993).

CHB-604: Physical Chemistry-IV

1. Quantum Mechanics of Simple Systems: Schrödinger's wave equation. Eigen functions and Eigen values and quantum mechanical operators. Expectation value of a physical quantity. Orthogonality of wave functions. The particle in a one dimensional box problem and its solutions. Particle in a three dimensional box. Degeneracy. Rigid rotor and Harmonic Oscillator.

Credits: 4

- 2. *Molecular Spectroscopy*: Region of electromagnetic spectrum. Emission and absorption spectra. Transition probabilities and selection rules. Width and intensity of spectral transitions Pure rotational spectra. Diatomic molecules-Rigid rotor & non-rigid rotors. Vibrational, rotational spectra of diatomic molecules. Harmonic oscillator-rigid rotor approximation. Anharmonicity effect. Normal modes of vibration. Infrared spectra of linear and bent AB₂ molecules. Electronic spectra of diatomic molecules. Vibrational structure. Franck-Condon principle.
- 3. Nuclear Magnetic Resonance Spectroscopy: Nuclear Magnetic Resonance spectroscopy. Chemical shifts. Spin-spin splittings. Relaxation times.
- 4. Molecular Statistics: The Boltzmann distribution. Maxwell distribution law for distribution of molecular speeds. The Maxwell-Boltzmann distribution law for the distribution of molecular energies. The partition functions. Thermodynamic quantities from partition functions. The Sackur-Tetrode equation for molar entropy of monatomic gases. Rotational and vibrational partition functions. The characteristic temperature. The calculation of Gibbs free energy changes and equilibrium constant in terms of partition functions.

Books Recommended

- 1. *Physical Chemistry*, K. J. Laidler and J. M. Meiser, 3rd Edition (International Edition, 1999), Houghton Mifflin Co., New York.
- 2. *Physical Chemistry*, I. N. Levine, 4th Edition (International Edition, 1995), Mc Graw-Hill Inc., New York.

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- 3. *Physical Chemistry A Molecular Approach*, D. A. Mc Quarrie and J. D. Simon, South Asian Edition (1998), University Science Books, Sausalito CA, by Viva Books, New Delhi.
- 4. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash, 4th Ed., Tata McGraw-Hill Publishing Company Ltd., New Delhi.

CHB-605: Inorganic Chemistry Practical

- 1. Preparation of coordination compounds.
- 2. Spectral and magnetic characterization of compounds

CHB-606: Organic Chemistry Practical

1. Preparation of the following compounds:
Suphanilic acid, dibenzal acetone, methyl orange, aspirin, m-dinitrobenzene from benzene, synthesis of azlactone, phthalimide,

2. Identification of organic functional groups by I.R. spectroscopy.

CHB-607: Practical Physical Chemistry

Credits: 2

Credits: 2

Credits: 2

- 1. Dissociation constants of weak acid, base.
- 2. Conductometric titration: acid-base.
- 3. Potentiometric titration: acid-base.
- 4. Kinetics of catalytic decomposition of H₂O₂.
- 5. Kinetics of acid-catalysed hydrolysis of sugar (chemical method).
- 6. Determination of relative strengths of two acids by studying the kinetics of acid-catalysed ester hydrolysis.
- 7. Kinetics of enzymatic reaction (starch-amylase system).

Note: Experiments may be added/deleted subject to availability of time and facilities.

CHB-608: Elective Paper Credits: 4

A. Atomic and Molecular Structure

- (1) <u>Atomic Structure</u>: The Schrödinger wave mechanics. The hydrogen atom. Atomic orbitals. Variation theorem. The He-atom, electron spin. Pauli Exclusion principle.
- (2) <u>Molecular Symmetry</u>: Symmetry elements and operations. Point groups. Symmetry species of H₂O molecule
- (3) <u>Molecular Structure:</u> Hydrogen molecule ion. MO approach. Diatomic MOs. VB approach. Hybridization

B. Application of Spectroscopic Techniques

- (1) <u>Infrared Spectroscopy</u>: Working and experimental considerations in spectral recording; Characteristic group frequencies; carbonyl frequencies; effect of structure: aldehydes, ketones; esters, amides, acid anhydrides, carboxylics acids, acid chlorides; effect of conjugation; cyclization; ambi-dentate ligands and metal carbonyls.
- (2) <u>Ultraviolet and Visible Spectroscopy</u>: Basic working principle and measurement technique; σ - σ *, π - π *, n- σ * and n- π * transitions, dienes and conjugated poly-enes; Woodward-Fieser rules; spectra of transition metal complexes (*d*-*d* transitions)
- (3) Mass Spectrometry: EI and CI techniques; isotope patterns, molecular ion, fragmentation

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- patterns. Mass spectra of simple compounds: (i) 2-hexane by β fragmentation and (ii) 4-n-butyltoluene by benzylic fission and McLafferty rearrangement.
- (4) <u>NMR Spectroscopy</u>: Working principle and method of measurement; factors influencing chemical shift, spin-spin splitting, PMR spectra of simple compounds of (i) benzyl alcohol (δ values) and (ii) ethyl bromide (δ and J values). CMR spectra of simple compounds and their interpretation (2-butanol, benzene, pyridine).

Books Recommended:

For Atomic and Molecular Structure

- 1. Physical Chemistry by G.M. Barrow, 5th Ed., Special Indian edition, 2007
- 2. Physical Chemistry by P.W. Atkins and J. De Paula, 8th Ed., Oxford University Press, 2006

For Spectroscopic Techniques and applications

- 1. W. Kemp, *Organic Spectroscopy*, 3rd Ed., (1991), Macmillan, London
- 2. J. R. Dyer, *Application of Absorption Spectroscopy of Organic Compounds*, Prentice Hall, New Delhi (1978).
- 3. D. H. Williams and I. F. Fleming, *Spectroscopic Methods in Organic Chemistry*, 4th Ed., (1988), Tata-McGraw Hill, New Delhi.
- 4. R. S. Drago, *Physical Methods in Inorganic Chemistry*, 1st Ed., (1971), Affiliated East-West Press, New Delhi

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