#### SUBJECT: CHEMISTRY UG

Class &	Dapar	Original	Now	Name of Paper	Credits
Class &	1 aper	Course	Course	Name of Laper	Creans
Semester		Course	Course		
		Code	Codes as		
			per OC-66		
TVDSo	Core	DSC 5	CHC 105	Physical Chemistry	4+2=6
	Core	DSC 6	CHC 106	Inorganic Chemistry	4+2=6
	Core	DSC 7	CHC 107	Organic Chemistry	4+2=6
	Discipline Specific	DSE 1	CHD 101	Basic Topics in Analytical	3+1=4
	Elective			Chemistry	
1.1.D.SC.			OR	OR	OR
Sem v					
			CHD 104	Essentials in Pharmaceutical	
				Chemistry	3+1=4
	Discipline Specific	DSE 2	CHD 102	Green methods and Safety	4+0=4
	Elective			Aspects in Chemistry	
	Core	DSC 8	CHC 108	Physical Chemistry	4+2=6
	Core	DSC 9	CHC 109	Inorganic Chemistry	4+2=6
	Core	DSC 10	CHC 110	Organic Chemistry	4+2=6
T.Y.B.Sc.	Discipline Specific	DSE 3	CHD 103	Selected Instrumentation in	4+0=4
Sem VI	Elective			Chemistry	
	Discipline Specific	DSE 4	CHP 101		4
	Elective = Project				
	(Compulsory)	(DSP)			

#### T.Y.B.Sc (Semester V & VI) for Bachelor of Science (Honours Programme)

## SEMESTER V CORE COURSE: CHC105 (06 Credits: Theory – 04, Practicals – 02) (PHYSICAL CHEMISTRY)

#### Theory : 60 Hours (04 Credits)

#### **SECTION A**

#### 1. Nuclear Chemistry I

Composition of the nucleus, nuclear binding forces and energy, nuclear stability, nucleon –nucleon forces and their equality, characteristics and theory of nuclear forces, nuclear models, radioactive disintegration, decay constant, half- life and average life, units of radioactivity, artificial radioactivity, detection and measurement of radioactivity, GM counter, semiconductor and proportional counter, Scintillation counter, characteristics of suitable scintillator. (numericals to be solved)

#### 2. Electrochemistry I

Ion-selective electrodes: Fixed-site membrane, mobile-site membrane, site-free membrane, construction of ion selective electrodes, applications of ion selective electrodes. Decomposition potential, experimental determination of decomposition potential, application of decomposition potential, overvoltage and overpotential, theory of overvoltage, experimental determination of overvoltage, factors affecting overvoltage, hydrogen overvoltage, oxygen overvoltage, metal overvoltage. Fuel cells; H<sub>2</sub>-O<sub>2</sub>, Molten carbonate fuel cell, Proton exchange membrane fuel cell, Solid oxide fuel cell, Electrochemical sensors, principle, advantages and applications.

#### **SECTION B**

#### 3. Quantum Chemistry I

Postulates of quantum mechanics, quantum mechanical operators and commutation rules, Schrodinger equation and its application to free particle and "particle in a box" (rigorous treatment) quantisation of energy levels, zero – point energy and Heisenberg Uncertainity principle, wave functions, probability distribution functions, nodal properites, Extension to two and three dimensional boxes, seperation of variables, degeneracy.

Angular momentum, Rigid rotator model of rotation of diatomic molecule. Schrodinger equation in Catesian and spherical polar (derivation not required). Seperation of variables,

#### 2

#### (20 Hours)

(10 Hours)

#### (16 Hours)

Spherical harmonics, Discussion of solution (Qualitative) required and their limitations, Refinement of two approaches (configuration interaction for MO, ionic terms in terms of VB), qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules. (HF, LiF).

#### 4. Molecular Spectroscopy I

#### (14 Hours)

Interaction of electromagnetic radiation with molecules and various types of spectra, Born Oppenheimer approximation.

Rotational Spectroscopy: selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degree of freedom for polyatomic molecules, modes of vibration, concept of group frequencies.

Vibration -rotation spectroscopy: Diatomic vibrating rotator, P, Q, R branches

Raman spectroscopy: Qualitative treatment of Rotational Raman effect, Effect of nuclear spin, Vibrational Raman spectra, Raman effect, Stokes and Anti-stokes lines, their intensity difference, Quantum and Classical theories of Raman effect rule of mutual exclusion principle.

#### **Text Books:**

- 1. J.N. Gurtu, Physical Chemistry Vol-III, A pragati edition.
- 2. N. B. Laxmeshwar, S. M. Malushte, A. S. Mulye, V. N. Kulkarni, Concepts of Physical Chemistry, Chetana Prakashan.
- 3. P. C. Jain, Monika Jain, Engineering Chemistry, 15<sup>th</sup> edition, Dhanpat Rai Publishing Co.

#### **Reference Books:**

- Barnwell, C.N. & McCash, E.M., Fundamentals of Molecular Spectroscopy, 4<sup>th</sup> Ed. Tata McGraw Hill, New Delhi (2006)
- 2. U. N. Dash, Nuclear Chemistry, S. Chand Publication
- H. J. Arnikar, Essentials of Nuclear Chemistry, New Age International Publishers, 4<sup>th</sup> Revised Edition
- 4. Gurdeep Raj, Advanced Physical Chemistry Goel Publication.

- 5. Chandra, A.K., Introductory Quantum Chemistry, Tata McGraw -Hill (2001).
- 6. House., J.E., Fundamentals of Quantum Chemistry, 2<sup>ND</sup> Ed. Elsevier: USA (2004)
- 7. Lowe. J.P. & Peterson., K., Quantum Chemistry, Academic Press (2005)
- 8. Kakkar., R., Atomic and Molecular Spectroscopy, Cambridge University Press (2015)

## SEMESTER V CHEMISTRY-LAB CORE COURSE: CHC105 (PHYSICAL CHEMISTRY)

#### Practicals: 60 Hours (02 Credits)

(10 x 6 Hours)

- 1. To study the kinetics of iodine clock reactions. [Ref. 1]
- 2. Using vibrational-rotational spectra of HCl and HBr molecules; [Ref. 1]
  - a. Assign the rotational lines to various transitions.
  - b. Calculate i) the value of  $B_0$  and  $B_1$ , for R and P branches of spectra.
    - ii) Vibrational frequency and
    - iii) Inter nuclear distance

c. Draw the vibrational-rotational energy levels and show the various transitions of R and P branches.

- 3. To determine the strength of mixture containing weak acid and salt of weak base by titrating against standard 0.1N NaOH solution conductometrically. [Ref. 4]
- 4. To determine the dissociation constant of a weak monobasic acid using pH metry. [Ref. 4]
- 5. To determine Standard Reduction Potential of Zn++/Zn and Cu++/Cu. [Ref. 4]
- 6. To determine the solubility product of AgCl. [Ref. 4]
- To determine the percentage composition and amount of halides from a mixture (any two halide) using standard 0.1N AgNO<sub>3</sub> solution. [Ref. 4]
- 8. To determine degree of hydrolysis and hydrolysis constant of a) CH<sub>3</sub>COONa and
  b) NH<sub>4</sub>Cl. [Ref. 4]
- 9. To study the adsorption of Acetic acid by charcoal and to verify Freundlich adsorption isotherm. [Ref. 4]
- 10. To determine the energy of activation of hydrolysis of ethyl acetate (unequal concentration) [Ref. 4]

#### Text Book:

1. Systematic experimental Physical Chemistry by W. Rajbhoj, T.K. Chondhekar, Anjali publication.

#### **Reference Books;**

1. Practicals in Physical Chemistry – a modern approach by P.S. Sindhu, published by

Macmillan India Ltd.

- 2. Practical Physical Chemistry by B. Viswanathan, P.S. Raghavan, published by Viva Books Private Ltd.
- 3. Senior Practical Physical chemistry by B.D. Khosla, V.C. Garg, Adarsh Gulati, published by R. Chand and Co.

2. Chemistry of halogens (8 Hours) General methods of preparation, structure, bonding and chemical properties of : i Interhalogens ii) Polyhalide ions iii) Oxyacids of halogens in different oxidation

states iv) Pseudohalogens.

#### 3. Noble Gases:

Occurrence and uses, inertness of noble gases, Clathrates; preparation properties and structure (VSEPR) of XeF<sub>2</sub>, XeF<sub>4</sub> and XeF<sub>6</sub>.

## SEMESTER V

#### **CORE COURSE: CHC106**

#### (06 Credits: Theory-04, Practicals-02)

#### (INORGANIC CHEMISTRY)

#### **SECTION A**

#### **1. Periodicity of Elements:**

**Theory: 60 Hours (04 Credits)** 

Detailed discussion of the following:

Properties of the elements with their trends in the periodic table.

- (a) Atomic radii (van der Waals)
- (b) Ionic radii and Covalent radii.
- (c) Effective nuclear charge, shielding or screening effect, Slater rules.
- (d) Ionization Energy, Successive ionization energies and factors affecting ionization energy.
- (e) Electron Affinity.
- (f) Electronegativity, Pauling's/ Mulliken's/ Allred and Rachow's. Calculation of Electronegativity (Paulings Method), Factors affecting Electronegativity.

(4 Hours)

(10 Hours)

#### 4. Inorganic Solid State Chemistry

Defects in solids, Point defects; Schottky and Frenkel defects, Colour centre, Extended defects and Non-stoichiometry.

Band Theory of solids: Band gaps, Metals, Insulators and Semi-conductors.

#### **SECTION B**

#### 5. Bonding in Co-ordination Compounds.

Werner's theory and its experimental verification Evidences for Covalent bonding in complexes; Stereochemistry of Co-ordination Compounds with different co-ordination Numbers

- A. Ligand Field Theory (Adjusted Crystal Field Theory) –Brief Introduction;
   Comparison of the CFT and MOT.
- B. Molecular Orbital Theory as applied to Octahedral Complexes.
   Stability of complexes and factors affecting stability.
- C. Molecular orbitals diagrams of  $[Ti (H_2O)_{6]}^{+3}$ ,  $[Fe (CN)_6]^{-3}$ ,  $[Fe F_6]^{-3}$  and  $[Co (NH_3)_6]^{+3}$  Complexes . Effect of  $\pi$  bonding on splitting parameter.

#### 6. Oxidation and Reduction.

Oxidation number, single electrode potential, Standard electrode potential and Electrochemical series. Energy cycle for electrode potential. Application of Electrochemical series to check feasibility of reaction. Hydrogen overvoltage and Oxygen overvoltage.

The use of reduction potentials, redox cycle, redox stability in water. The diagrammatic presentation of potential data - Frost, Latimer and Poubaix diagrams. Principles involved in the extraction of the elements.

#### 7. Selected Topics:

**A) Nanochemistry:** Introduction to nano particles, their properties, carbon nanotubes, SWCNT, MWCNT, different types of nanomaterials and their applications.

#### (8 Hours)

#### (8 Hours)

(5 Hours)

#### (12 Hours)

#### **B)** Bio-inorganic Chemistry

#### (5 Hours)

Overview, essential and trace elements in biological processes, Metalloporphyrins with special reference to haemoglobin and myoglobin. The role of Model systems, The alkali and alkaline earth metals, Metalloenzymes, Nitrogen fixation: Bacterial nitrogenase system (The biological nitrogen cycle).

#### Text books:

- 1. J. D. Lee, *Concise Inorganic* Chemistry, 5<sup>th</sup> Edn. Wiley India.
- B. R. Puri, L. R. Sharma and K. C. Kalia, *Principles of Inorganic Chemistry*, 33<sup>rd</sup> Edn.

#### **Reference books:**

- F. Albert Cottton, Geoffrey Wilkinson and Paul L. Gaus, *Basic inorganic chem.* 3<sup>rd</sup> Edn. Wiley India
- James E. Huheey, Ellen A. Keiter, Richard L.Keiter and Okhil K. Medhi, Inorganic Chemistry, Principles of Structure and Reactivity. 4<sup>th</sup> Edn. Pearsons
- K. V. S. Laxmi Devi, N. C. Patel, S.S. Dhume, A. Venkatachalam, S. P. Turakhia, Chhaya Dixit and R. A. Mirji, College Inorganic Chemistry for T.Y. B. Sc. 21<sup>st</sup> Edn, Himalaya Publishing House.
- 4. Solid State Chemistry, Third edition By- Lesley E. Smart, Elaine A. Moore, Pub-Taylor and Francis.
- 5. D. E. Shriver, P.W. Atkins and C.H. Langford, *Inorganic Chemistry*, Oxford.
- 6. G.D. Tuli, S. K. Basu and R.D. Madan, Advance inorganic chemistry, Satya Prakash, S. Chand Publication.
- 7. F. A. Cotton, Chemical Applications of Group Theory, Wiley India
- P.K Bhattacharya ,Group Theory and its Chemical Applications Himalaya Publications.

#### SEMESTER V CHEMISTRY- LAB CORE COURSE: CHC106 (INORGANIC CHEMISTRY)

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#### Practicals: 60 Hours (02 Credits)

#### **Gravimetric Estimations**

- 1. To estimate the amount of Al as  $Al_2O_3$  in the given solution of aluminium sulphate.
- 2. To estimate the amount of Fe as  $Fe_2O_3$  in the given solution of ferric chloride containing barium chloride and free HCl.
- 3. To estimate the amount of nickel as Ni-DMG in the solution of nickel chloride containing copper chloride and free HCl.
- 4. To estimate the amount of barium as BaCrO<sub>4</sub> in the solution of barium chloride containing ferric chloride and free HCl.
- 5. To estimate the amount of Zinc as  $Zn_2P_2O_7$  in the given solution of zinc sulphate containing copper sulphate and free  $H_2SO_4$ .

#### **Inorganic Preparations**

(Percentage yield expected)

- 6. Preparation Potassium trioxalatoferrate (III).
- 7. Preparation of potassium trioxalatoaluminate(III).
- 8. Preparation of Tristhioureacopper(I) sulphate
- 9. Guignet's green (hydrated chromium oxide)
- 10. Cobalt blue (azure)

## [Note : Pre-sessions are expected to explain the principle, procedure and calculations of each experiment]

#### Text book:

1. G.H. Jeffery, J. Bassett, J. Mendham, R. C. Denney, Vogel's Textbook of Quantitative Chemical Analysis, 5<sup>th</sup> Edn. ELBS

#### **Reference books:**

1. J. Mendham, R. C. Denney, J.D. Barnes, M. Thomas, B. Sivasankar, Vogel's Textbook of Quantitative Chemical Analysis, 6<sup>th</sup> Edn. Pearson

2.S. Ratan, Experiments in Applied Chemistry, 3<sup>rd</sup> Edn. S.K. Kataria & Sons

3.O. P. Pandey, D. N. Bajpai and S. Giri, Practical Chemistry, Revised Edn. S. Chand.

## SEMESTER V **CORE COURSE: CHC107** (06 Credits: Theory-04, Practicals-02) (ORGANIC CHEMISTRY)

#### **Theory: 60 Hours (04 Credits)**

#### **SECTION A**

#### 1. Aromaticity, Aromatic hydrocarbons and Reactivity (6 Hours)

Huckel's rule of Aromaticity (4n+2) Rule, 4n Rule for antiaromaticity, Electrophilic Aromatic substitution (w.r.t Benzene): Mechanism of Nitration, Sulphonation, Halogenation, Friedel - Crafts alkylation and acylation. Reactivity and orientation of activating, deactivating groups (ortho, para and meta effects). Nucleophilic aromatic substitution of Aryl halides (SNAr mechanism).

#### 2. Alkaloids

Ziesel's Method, Herzig-Meyer's method, Hoffman's exhaustive methylation method. Structure elucidation of Nicotine, Papaverine and Hygrine. Synthesis of Nicotine from Succinimide. Synthesis of Papaverine using Bischler-Napieralski reaction. Synthesis of Hygrine from Pyrrole.

#### 3. Spectroscopic methods in Organic Chemistry

#### Infra Red Spectroscopy:

Principle of I.R Spectroscopy (Hooke's law), types of molecular vibrations (Stretching and bending). Source, instrumentation and working of I.R spectrophotometer. Functional group region and Fingerprint region. Applications of I. R. Spectroscopy: Functional group analysis, detection of purity of sample, establishing the identity of an unknown molecule, Effect of H-bonding, conjugation, resonance and ring size on IR absorptions. To study the progress of a reaction. Problems based on I.R. spectroscopy (ketone, aldehyde, ester, acid & alcohol).

Nuclear Magnetic Resonance Spectroscopy:

#### (6 Hours)

(18 Hours)

Basic Principles of 1H NMR spectroscopy, Number of signals (Homotopic, Enantiotopic, diastereotopic protons). Position of signals, Chemical shift: Reference standard, Solvent effect, Shielding and deshielding effect, anisotropic effects in alkenes, alkynes, aldehydes, aromatic compounds, factors affecting chemical shift. Intensity of signals: Peak area and proton counting. Spin-Spin coupling: Coupling constant (J). Interpretation of NMR spectra of simple compounds. (acetone, acetaldehyde, toluene, ethyl bromide, anisole, acetic acid, t-butylbenzene, 2-butanone, propene). Simple problems based on NMR spectral data for identification of molecule.

Carbon-13 Nuclear Magnetic Resonance Spectroscopy and Mass Spectrometry:

Principle of <sup>13</sup>C spectroscopy. Number of signals: Proton coupled and decoupled spectra (off-resonance). Position of signals. Factors affecting position of signals (hybridisation). Problems based on <sup>13</sup>C spectroscopy.

Principle, theory, instrumentation of Mass spectrometry. Base Peak, Molecular ion, Metastable ion. Fragmentation pattern for alkanes. Fragmentation pattern of ketones:  $\alpha$ -cleavage and McLafferty rearrangement. Isotopic effect of alkyl halides.

#### **SECTION B**

#### 4. Chemistry of Heterocyclic Compounds

#### (18 Hours)

Definition of heterocyclic compounds: Organic compounds containing oxygen, sulphur, nitrogen. Classification with examples for three, four, five and six membered heterocycles. Structure, resonance, stability and industrial source of furan, pyrrole, thiophene and pyridine. Preparation of furan, pyrrole and thiophene using Paal Knorr Synthesis. Reactivity of furan, pyrrole and thiophene: Electrophilic substitution at 2/5 position. Preparation of pyridineusing Hantzsch synthesis. Reactivity of pyridine: Electrophilic substitution at 3 position, Nucleophilic substitution at 2 and 4 position. Definition of bicyclic heterocycles with examples. Structure, resonance, stability and industrial source of indole, quinoline, isoquinoline. Preparation of indole using Fischer indole synthesis. Reactivity of Indole: Electrophilic substitution at 3 position. Skraup synthesis of quinoline and Bischler Napieralski synthesis of isoquinoline. Reactivity of quinoline and isoquinoline: Electrophilic substitution at 5/8 position, Nucleophilic

substitution at 2 and 4 position. Oxidation and Reduction of quinoline and Isoquinoline.

#### 5. Vitamins and Hormones

Structure elucidation of Vitamin A , Vitamin C , Thyroxine and Adrenaline. Synthesis :Vitamin A from  $\beta$ -ionone ,Vitamin C from xylose , Adrenaline from Catechol and thyroxine from tyrosine.

#### 6. Dyes

Classification of dyes: Acidic, basic, azo, reactive, Vat, mordant, direct, disperse with one example and structure of each class. Reasons for colour of some molecules: Resonance effect in p-nitroaniline and nitrobenzene, conjugation effect in  $\beta$ -carotene and graphite. Synthesis and chemistry of phenolphthalein, congo-red, crystal violet, methyl orange.

#### **Text books :**

- 1. I.L.Finar, Organic Chemistry Vols I and II, Orient Longman
- 2. Morrison and Boyd, Organic Chemistry; 6<sup>th</sup> Edn. Prentice Hall India
- J. March, Advanced Organic Chemistry: Reaction, Mechanism and Structure, Wiley, 2010, 4th Ed.
- P.S. Kalsi, Spectroscopy of Organic compounds, New Age International Pub. Ltd. & Wiley Eastern Ltd., Second edition, 1995.

#### **Reference books :**

- 1. Francis Carey, Organic Chemistry, 10<sup>th</sup> Edition.
- 2. Paula Yurkanis Bruice, Organic Chemistry; 3rd Edn. Pearson Education Asia
- 3. Silverstein, Bassler and Morill, Spectrometric Identification of Organic Compounds.
- 4. J. Clayden, N. Greeves, S. Warren & Wothers, Organic Chemistry,

Oxford University Press, 2012, 2nd Ed.

2. I.L. Finar Stereochemistry and Chemistry of Natural products, ELBS,

Longmans, 1963, Vol. 2, 3rd Ed.

- 3. E.S. Gould et al., Mechanism and structure in Organic Chemistry, 1965
- 7. F. A. Carey, Organic Chemistry, 2000, 4th Ed.

#### 14

#### (6 Hours)

#### (6 Hours)

- 8. S.H. Pine, Organic Chemistry, McGraw-Hill International Edn. 2010, 5thEd.
- F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Part A and Part B. Plenum Press, Springer, 1977
- J. M. Harris & C.C. Wamser, Fundamentals of Organic Reaction Mechanisms, John Wiley & Sons. Inc. 1976
- F.M. Menger, D.J. Goldsmith & L. Mendell, Organic Chemistry, A concise approach, 1975, 2nd Ed.
- Applications of Absorption Spectroscopy of Organic compounds, J. R. Dyer, Prentice Hall of India, 1987.
- V.M. Parikh, Absorption spectroscopy of organic Molecules, Addison Wesley Longman Publishing Co., 1974.
- D.H Williams & I. Fleming, Spectroscopic methods in organic chemistry, 6<sup>th</sup> Ed., Tata Mcgraw Hill Education, 2011.
- 15. William Kemp, Organic spectroscopy, 3rd Ed., Palgrave Macmillan, 1991.
- R. O. C. Norman and J. M. Coxon, Principles of Organic Syntheses, 3rd Ed., CRC Press Inc, 1993.
- Heterocyclic Chemistry, J A Joule and G F Smith, ELBS, Advances in Heterocyclic Chemistry, Edited by A R Katritzky etal, Vol. 1 to 50, Academic Press.
- 18. Synthetic dyes, Gurdeep Chatwaal, Himalaya Publishers

## SEMESTER V CHEMISTRY LAB CORE COURSE: CHC107 (ORGANIC CHEMISTRY)

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## Laboratory Course : 60 hours (02 Credits)

#### 1. Organic Preparations (Two steps): (Any 5)

#### Synthesis, yield, recrystallisation and Melting Point.

- i) Nitrobenzene to m-nitroaniline
- ii) Phthalimide to 2-iodobenzoic acid
- iii) Acetanilide to p-nitroaniline
- iv) Benzamide to m-nitrobenzoic acid
- v) Benzoin to benzilic acid
- vi) Acetophenone to acetanilide
- vii) Benzophenone to benzanilide

#### Ref. 1, 3, 4, 8

#### 2. Organic Estimations (Any 3)

- a) Acid+ Amide
- b) Acid + Ester
- c) Estimation of the number of acetyl groups in an acetyl ester. (Triacetyl glycerol, Hexaacetyl mannitol or Pentaacetyl glucose) (Any One)
- d) Estimation of nitro group by reduction using stannous chloride.

Ref. 4, 7, 8

#### 3. Synthesis of dyes

- a) Diazoaminobenzene
- b) Picric acid

#### Ref. 1, 2, 7

#### 4. Interpretation of Infra Red, and proton NMR spectra.

- a) IR spectra of the following: aldehyde, alcohol, ketone, carboxylic acid, amine, nitrile.
- b) Proton NMR of simple organic compounds(6 compounds)

Ref. 6, 9, 10

#### 5. Identification and Separation of following Organic binary mixtures.

Water insoluble -water insoluble

(Acid-Base, Acid-Phenol, Base-Neutral, Acid-Neutral, Phenol-Base, Phenol-Neutral)

Water soluble- water insoluble

(Acid-Acid, Acid-Neutral, Neutral-Neutral)

Liquid-Liquid (2 mixtures)

Solid-liquid (2 mixtures)

# (Note: Examiners should evaluate the experiments performed during the regular practicals.)

#### **Text books**

- 1. A.I. Vogel, A.R. Tatchell , B. S. Furniss, A.J. Hannaford, *Vogel's Textbook* of *Practical Organic Chemistry*, 5th Ed., Prentice Hall; 2011.
- 2. Practical organic chemistry, F G Mann and B C Saunders, Orient Longman, 4th ed.

#### **Reference books:**

- 1. D. Pasto, C. Johnson and M. Miller, *Experiments and Techniques in Organic Chemistry*, 1st Ed., Prentice Hall, 1991.
- L.F. Fieser, K.L. Williamson "Organic Experiments" 7th edition D. C. Heath, 1992.
- K.L. Williamson, K.M. Masters, *Macroscale and Microscale Organic Experiments*, 6th Edition, Cengage Learning, 2010
- 4. R.K. Bansal, *Laboratory Manual in Organic Chemistry*, New Age International, 5th Edition, 2016.
- 5. Morrison and Boyd, Organic Chemistry, 6th Edition, Prentice Hall , Indsia
- 6. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*, Universities Press.
- 7. Silverstein, Bassler and Morill, Spectrometric Identification of Organic Compounds.

 S. Kalsi, Spectroscopy of Organic compounds, New Age International Pub. Ltd. & Wiley Eastern Ltd., Second edition, 1995.

## SEMESTER V DISCIPLINE SPECIFIC ELECTIVE: CHD101 (04 Credits: Theory - 03, Practical - 01) (BASIC TOPICS IN ANALYTICAL CHEMISTRY)

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#### Theory: 45 Hours (03 Credits)

#### **1. Introduction:**

Scope and importance of analytical chemistry, chemical analysis and analytical chemistry. Classification of instrumental methods, analytical process (steps involved in chemical analysis): defining the problem, sampling, separation of desired components, actual analysis, presentation and interpretation of results.

#### 2. Quantitative analysis:

- A. Principles of volumetric analysis: Theories of acid-base, redox, complexometric, iodometric and precipitation titrations choice of indicators for these titrations.
- B. Principles of gravimetric analysis: precipitation, coagulation, peptization, coprecipitation, post precipitation, digestion, filtration and washing of precipitate, drying and ignition.

#### 3. Sampling Techniques:

Terms encountered in sampling: the population or the universe, Sample, Sampling unit, increment, the gross sample, the sub sample, Analysis sample, Bulk ratio, Size to weight ratio, Random sampling, Systematic sampling, Multistage sampling, Sequential sampling. Sampling of Gases, Liquids and Solids. Preservation, storage and preparation of sample solution.

#### 4. Evaluation of analytical data.

Significant figures and rounding off, accuracy and precision Errors: determinate and indeterminate error, constant and proportionate errors, minimization of errors.

#### (3 Hours)

(8 Hours)

(4 Hours)

(10 Hours)

Measures of central tendency and dispersion. Standard deviation, Gaussian distribution curve and its characteristics, Histogram and Frequency polygon. Confidence limit. Test of significance: Students t, F test, Rejection of the results: 2.5d & 4d rule and Q test. Linear least squares and Method of averages (Numerical problems are expected to be solved)

#### 5. Solvent Extraction

Basic Principle, percentage extraction, role of complexing agents in solvent extraction, separation factor, types of extraction (continuous, batch) (Numerical problems are to be solved).

#### 6. Chromatography:

Principles Classification of chromatographic techniques

- (A)Column chromatography: Principle, experimental details, theory of development, factors affecting column efficiency and applications.
- (B) Paper and thin layer chromatography: Principles, techniques and applications of paper and thin layer chromatography.
- (C) Ion exchange chromatography: Principles, classification of ion exchange materials, Nature of exchanging ions, Ion exchange capacity, applications in analytical chemistry.

#### 7. Electroanalytical methods:

Electrogravimetric analysis: Introduction, principles, instrumentation, Electrolysis at constant current, apparatus, determination of copper by constant current electrolysis. Coulometry: Introduction, constant Current measuring device, Hydrogen-Oxygen coulometer, Silver coulometer. General characteristics of coulometric method, applications of coulometry in Neutralization, complexation, precipitation and redox titrations.Polarography: Introduction, Basic principles of instrumentation, Deposition potential, Dissolution potential, Polarisation of electrode, Polarographic wave, Ilkovic equation, Supporting electrolytes, Interference of oxygen, Applications of polarography – inorganic and organic.

#### (9 Hours)

#### (**4 Hours**) olvent extra

#### (7 Hours)

#### Text books :

1. Baliga and Shetty, College Analytical Chemistry, 15<sup>th</sup> edition, Himalaya Publishing House, 2004

2. K. Raghuraman, D. V. Prabhu, C. S.Prabhu and P. A. Sathe, 5<sup>th</sup> Edn. Sheth Publishers Pvt.Ltd.

#### **Reference Books:**

1. G. D.Christan Analytical Chemistry by, 5<sup>th</sup> edition Wiley publications.

2. G. Chatwal and S. Anand, Instrumental Methods of Chemical Analysis 5<sup>th</sup> edition (reprint 2003), Himalaya publication.

3. Vogels Textbook of Quantitative Inorganic Analysis 4<sup>th</sup> edition ELBS.

4. Willard, Meritt and Dean. Instrumental Methods of Analysis

5. Skoog and Leary, Principles of Analytical Chemistry 4<sup>th</sup> International edition.

6. B.K. Sharma. Instrumental Methods of Chemical Analysis: Goel Publishing House, Meerut

7. Mendham, J. Vogel's Quantitative Chemical Analysis( 6th Edition ) Pearson.

## SEMESTER V DISCIPLINE SPECIFIC ELECTIVE: CHD101 (04 Credits: Theory -03, Practical -01)

#### (BASIC TOPICS IN ANALYTICAL CHEMISTRY)

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#### PRACTICALS: 30 Hours (1Credit)

- 1. Determination of iron by salicylic acid by colorimetry.
- 2. Determination of nitrite in water by colorimetry.
- 3. Separation of organic compounds by TLC. (Demonstration)
- 4.  $Zn^{2+}/Mg^{2+}$  separation by an anion exchanger & volumetric estimation of Magnesium with standard EDTA.
- 5.  $Zn^{2+}/Mg^{2+}$  separation by an anion exchanger & volumetric estimation of Zinc with standard EDTA.
- 6. Estimation of Na<sup>+</sup> in NaCl by cation exchange resin using standard NaOH.
- 7. Estimation of Ca in calcium tablet by oxalate method and titration with KMnO<sub>4</sub>.
- 8. Determination of hardness of water by EDTA i.e. estimate Ca as CaCO<sub>3</sub> and report analysis in ppm. (The candidate should record more than 5 observations and carry out statistical analysis to find out mean, median, range, standard deviation, absolute error, relative error and possibly Q test.

#### **Reference Books:-**

- 1. Practical Chemistry by Dr O.P.Pandey, D.N.Bajapai, Dr. S.Giri. (S Chand Publications)
- 2. Experiments in Applied Chemistry by Dr. Sunita Rattan.
- 3. Vogel's Qualitative Inorganic Analysis revised by G. Svehla, Pearson Education, 2002
- 4. Mendham, J. Vogel's Quantitative Chemical Analysis (6th Edition ) Pearson

## SEMESTER V DISCIPLINE SPECIFIC ELECTIVE COURSE: CHD104 (4 Credits: Theory-03, Practicals-01) (ESSENTIALS IN PHARMACEUTICAL CHEMISTRY)

#### Theory: 45 Hours(03 credits)

#### **1.** General Introduction to Pharmaceutical Chemistry: (4 Hours)

Importance of Chemistry in Pharmacy. Important terminologies: Pharmaceutical Chemistry, Pharmacokinetics, Pharmacodynamics, Pharmacophore, Pharmacopoeia, Pharmacognosy, Toxicology, Materia Medica, Drug. Drug Product formulation, drug dosage forms, routes of drug administration: Oral, Parenteral, Enemal, Topical (Advantages and Disadvantages).

Assay of drugs. Chemical Assay (Titrimetric and Instrumental methods), Biological assay : Principles of bioassay, methods of bioassay, Invitro and Invivo assay.

#### 2. Physicochemical properties of drugs and drug metabolism (5 Hours)

Effect of solubility, partition coefficient, ionisation constant, hydrogen bonding, chelation, electronic effect, steric effect, surface activity and cis-trans isomerism on the pharmacological action of drugs. Drug Metabolism: Definition, Phase I drug metabolism: Oxidation, Reduction and Hydrolysis. Phase II drug metabolism: Conjugation reactions. Factors on which drug metabolism depends.

#### **3.** Nomenclature of drugs and structure activity relationship (4 Hours)

Drugs -Nomenclature, Naming of drugs: code number, chemical name, brand name/trade name/optical name/common name, synonyms. Examples Aspirin, Ibuprofen, Chloroquine, Mebendazole,Caffeine, Propranolol, Methyl Dopa. Effect of various functional groups on the chemical activity of drugs (acidic, hydroxyl, amino, thiol, acetyl, aldehyde, cyano, halogen, alkyl, ether, ester).

#### 4. Introduction to Drug Design

Development of new drugs: Introduction, procedure followed in drug design, the search for lead compounds, molecular modification of lead compounds, prodrugs and soft drugs, prodrug; introduction, prodrug formation of compounds containing various chemical groups, multiple prodrug formation, soft drugs; design of soft drugs. Design of Enzyme Inhibitors, 9-alkylpurines, 9-mercaptopurines and allopurines, active side directed irreversible enzyme inhibition, suicide enzyme inactivators.

#### 5. Definition and Classification with structure of the following drugs :

#### Anti Infective agents:

#### (6 Hours)

Antiseptics and Disinfectants: Alcohols, substituted phenols, DDT, p-hydroxy-benzoic acid esters, Chloramine-T, 8-hydroxy quinoline derivatives, Acridine derivatives, Mercurials like (Mercurochrome) and Nitrofurantoin derivatives, Bromopal, Halazone. Synthesis, use and side effects of DDT and Halazone.

Antimycobacterial agents (Antitubercular and Antileprotic drugs) Aminosalicylic acid, Isoniazid, Pyrazinamide, Ethambutol, Dapsone, Clofazimine and important drug combinations. Synthesis, use and side effects of Isoniazid and Ethambutol.

Antimalarials: Life cycle of parasite, drug acting on different stages- Quinine, Mefloquine, Chloroquines, Trimethoprim. Antiamoebics: Metronidazoles, Diloxanides,. Anthelmintics:Piperazine, Niclosamide, Mebendazoles, Praziquantels. Synthesis, use and side effects of Metronidazole and Niclosamide.

Antifungal: Antibiotics like Tolnaflates, Clotrimazoles. Antivirals including drugs acting on HIV: Idoxuridiness, Amantadine Hydrochlorides. Synthesis, use and side effects of Clotrimazole and Idoxuridiness.

#### 6. Antineoplastics, Sulfonamides, Hypoglycemics, Diagnostic agents and Diuretics: (5 Hours)

6-Mercaptopurines, Thiotepa, Chlorombucils, Doxorubicin, Cis-platin, Sulfacetamide, Sulfamethoxazoles,: Insulin and various sulfonyl ureas like tolbutamide, Tolazamides, Metformin, Saccharin. Iodoxyls, aminohippuric acid. Sulfonamides – Acetazolamides, Benzothiadiazones –Hydrochlorthiazide, Ethacrynic acid, Theophylline.

Synthesis, use and side effects of sulphacetamide, thiotepa.

#### (5 Hours)

7. Analgesic, antipyretics, anti-inflammatory and antibiotic drugs: (4 Hours) Definition and Classification with structure of the following drugs: Aspirin, Acetaminophen, Oxyphenabutazone, Ibuprofen, Naproxen, Diclofenac. Narcotic analgesic agents: Morphine. Non-narcotic analgesic agents: Dextropropoxyphene. Antibiotics: Penicillin and semisynthetic pencillins and Chloramphenicol, Clavulanic acid. Synthesis, use and side effects of Aspirin, Ibuprofen.

#### 8. Cardiovascular and Parkinsonism drugs: (4 Hours)

Antianginal drugs: Angina pectoris condition-Isosorbide dinitrate, Vasodilators: Cylandelate, Antiarrythmic agents: Cardiac Arrythmia condition Verapamil, Antihypertensive agents: hydralazine, Methyl dopa, Coagulants and Anticoagulants: Vitamin K, Coumarin derivatives like Warfarin, Dicoumarol. Antilipidemics: Atherosclerosis condition, Clofibrates, Nicotinic acid, Boxidines. Drugs used in Parkinsonism: Levodopa, Amantadine hydrochloride. Drugs for Alzheimer's iseases: Velnacrine. Synthesis, use and side effects of Methyl Dopa and Warfarin.

#### 9. Central Nervous System Drugs

#### (3 Hours)

Local anaesthetics: Benzocaines, Lidocaine. General Anaesthetics: Ether, Nitrous oxide, Halothane, Ultra short acting Barbiturates-Thiopental sodium. Drugs acting on the central nervous system: a] Hypnotics and sedatives: Phenobarbital
b] Drugs acting as anticonvulsants: Phenytoin, Phenobarbital, Carbamezepine. c]
Psychotherapeutic agents: Phenothiazines such as Chloropromazine, Diazepam. d] CNS stimulants: Nikethamide, Caffeine. Synthesis, use and side effects of Phenytoin, Nikethamide.

10. Drugs acting on cholinergic and adrenergic nervous system: (3 Hours)
Drugs acting on cholinergic nervous system Methacholine, Neostigmine, Dicyclomine,
Tropicamide. Drugs acting on adrenergic nervous system: Methyldopa, Pragyline,
Epinephrine, Propanalol, Metoprolol. Synthesis, use and side effects of Bethanechol and
Propranolol.

# 11. Antihistaminics and antiemitics and antiulcer drugs:(2 Hours)Chloropheniramine, Cyclizine, Promethazine, Omeprazole, Ranitidine. Synthesis, useand side effects of Chloropheniramine, Promethazine.

#### Text books:

- Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, 8th edition Edited by Robert F. Doerge, J. B. Lippincott Company, Philadelphia, USA.
- 2. Harikishan, V.K. Kapoor: *Medicinal and Pharmaceutical Chemistry*, Vallabh Prakashan, Pitampura, New Delhi.
- 3. Medicinal Chemistry, D. Shriram, P. Yogeshwari, Pearson Education, 2007.
- 4. Medicinal Chemistry, Chatwal, Himalaya Publishing house, 2002.
- 5. Textbook of Pharmaceutical Chemistry by ,Jayshree Ghosh, S. Chand & company Ltd.
- 6. Pharmaceutical Chemistry by Dr. S. Lakshmi, Sultanchand & Sons.

#### **References books:**

- 1. G.L. Patrick: Introduction to Medicinal Chemistry, Oxford University Press, UK.
- 2. William O. Foye, Thomas L., Lemke , David A. William: *Principles of Medicinal Chemistry*, B.I. Waverly Pvt. Ltd. New Delhi.
- Lednicer and Meischer, Organic Chemistry of Drug Synthesis. Vol. I to III. John Wiley & Sons, 2005.
- 4. Burger's Medicinal Chemistry, Part I and II, 4th edition, Edited by M. E. Wolff, John Wiley.
- Principles of Medicinal Chemistry, W. O. Foye, 3rd edition, K. M. Varghese and Co., Bombay.
- 6. Burgers Medicinal Chemistry and Drug Discovery, Vol. I, 6th edition, Edited by Donald J. Abraham, John Wiley and Sons, New Jersey, 2003.

#### SEMESTER V CHEMISTRY - LAB DISCIPLINE SPECIFIC ELECTIVE COURSE: CHD104 4 Credits: Theory-03, Practicals-01) (ESSENTIALS IN PHARMACEUTICAL CHEMISTRY)

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#### **Practicals: 30 Hours ( 01 Credit)**

- 1) Indian Pharmacopoeia Monograph of Aspirin and Purified water. (Any One)
- 2) Spectrophotometric assay of Metformin hydrochloride and Albendazole.
- Synthesis of Sulphacetamide, Dilantin, Paracetamol, 7-hydroxy-4-methyl coumarin. (Any 3)
- 4) TLC identification of analgesic drugs comparison of bulk drugs with branded drugs.

#### **Reference books :**

- 1. Indian Pharmacoepoiea. Latest edition.
- 2. A.I. Vogel, A.R. Tatchell, B. S. Furniss, A.J. Hannaford, *Vogel's Textbook* of *Practical Organic Chemistry*, 5th Ed., Prentice Hall; 2011.

## SEMESTER V DISCIPLINE SPECIFIC ELECTIVE: CHD102 (04 Credits: Theory 04)

#### (GREEN METHODS AND SAFETY ASPECTS IN CHEMISTRY)

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#### Theory: 60 Hours (04 credits)

#### **SECTION A**

#### 1. Green Chemistry

Introduction. Why there is a need for green chemistry? A brief overview of twelve green chemistry principles as proposed by Paul Anastas and John Warner. Explanation with examples, with special emphasis on atom economy, designing of less hazardous substances, reducing toxicity, use of greener solvents, catalysis, Energy efficiency, alternative sources of energy, accident prevention and green Chemistry for better sustainability. Brief on green chemistry institutes and organizations in the world.

#### 2 Green techniques in Chemistry

#### Greener solvents: Water as solvent-Diels Alder Reaction, supercritical liquidsextraction of D-limonene from orange pill, ionic liquids and deep eutectic solventsproperties- one application. Solvent free reaction: Grinding techniques.- Aldol condensation between 3,4-dimethoxybenzaldehyde and 1-indanone. and Ball milling techniques in synthesis. Catalysts: Definition: Solid supported reagents- NaBH4-Alumina and PCC-silica. natural catalysts-Thiamine hydrochloride, L-Proline. Phase transfer catalysis: Phase Transfer catalyst, Mechanism of PTC, Advantages and application in Chemistry-Using 18-crown-6 ether or ammonium salt. Microwave and Ultrasound techniques: Principles and advantages, Green synthesis of metallophthalocyanine complexes by Microwave method. Preparation of Grignard reagent by ultrasonication method. Solid-solid synthesis of Schiff's base. (p-toluidine and o-vanillin). Green preparation of 1-acetylferrocene and bis(acetylacetanato) copper (II).

27

#### (10 Hours)

#### (10 Hours)

#### 28

#### **3** Real world Cases in Green Chemistry

Surfactants for carbon dioxide – Replacing smog producing and ozone depleting solvents with CO<sub>2</sub> for precision cleaning and dry cleaning of garments. Designing of environmentally safe marine antifoulant. Right fit pigment: Synthetic azo pigments to replace toxic organic and inorganic pigments. An efficient, green synthesis of a compostable and widely applicable plastic (polylactic acid) made from corn. Greening of acetic acid manufacture, EPDM rubbers and Vitamin C. Eco-friendly pesticides.

#### **SECTION B**

#### 4 Introduction to Laboratory Safety

Risks in a Chemical Laboratory, Health Effects Due to "Hazardous" Chemical Exposure (How Does One Determine the Hazards Associated with Specific Chemicals?, Exposure Routes, Toxicity Risk Assessment), Personal Protective Equipment (PPE) Proper Attire (Eye/Face Protection, Lab Coats, Gloves, Respirators, Disposal/Removal of PPE), Emergency Equipment Safety Showers/Eye Washes.

#### **5** Laboratory Emergencies

Spills and Fires, Handling the Accidental Release of Hazardous Materials, Spill Containment and Clean-up, Leaking Gas Cylinders, Fires. Fire Extinguisher (how they work, types), Risk Assessment. Chemical Hazards, The New Safety Data Sheets (SDS) versus the Old Material Safety Data Sheets (MSDS), Assessment of Chemical Toxicity, Toxic Hazards (Dose, Risk Assessment, Types of Toxins, Flammable Hazards, Flammability Characteristics, Flammability Classes, Causes of Ignition, Reactive Hazards, Explosives).

#### 6. Waste Handling and Laboratory equipment

Characterization of Waste, Collection and Storage (Lids, Leaks, Labels, Location, Containers). Consequences of Mixing Incompatibles. Solid Wastes (Chemicals, Broken Glass, Sharps, Cylinders, Pick-up). Special Cases. Hazardous Waste Minimization. Laboratory Equipment. Working with Electricity, Working with Water (liquid)dependent Equipment (Hazards, Proper Use, Heating Baths), Working with High Pressure/Vacuum, Working with Vacuum Pumps, Working with Stirring and Mixing

#### (10 Hours)

(10 Hours)

#### (10 Hours)

#### (10 Hours)

Devices, Working with Heating Devices (Variacs, Oil, Salt, SandBaths, Microwave Oven).

#### Text books:

- 1. Vogel's text book of Practical Organic Chemistry, ELBS Publishers, 1996.
- 2. Anastas, P.T. & Warner, J.K. *Green Chemistry- Theory and Practical*, Oxford University Press (1998).
- 3. Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. *Green Chemistry Experiments: A monograph* I.K. International Publishing House Pvt Ltd. New Delhi, Bangalore.
- Green Chemistry: Environmentally Benign Reactions, V. K. Ahluwalia, Anne Books India, New Delhi, 2006.

#### **Reference books:**

- 1. Cann, M.C. & Connely, M.E. *Real-World cases in Green Chemistry*, American Chemical Society, Washington (2000).
- 2. Phase Transfer Catalysis, Waber and Gokel, springer-verlag, 1977.
- 3. Organic Synthesis-Special Techniques, V.K. Ahluwalia and R. Aggarwal, Narosa Publishing House, New Delhi, 2001.
- Kappe, C. O. & Stadler, A. Microwaves in Organic and Medicinal Chemistry (Wiley-VCH, Weinheim) 2005.
- 5. New trends in Green Chemistry, V.K.Ahluwalia and M.Kidwai, Kluwer Academic Publishers,2004.
- Laboratory Safety for Chemistry students, Robert H. Hill, David C Finster, Wiley, July, 2010.
- 7. Laboratory safety: Theory and Practice, 1<sup>st</sup> Edition, Elseviers.

#### SEMESTER VI CORE COURSE: CHC108 (06 Credits: Theory – 04, Practicals – 02) PHYSICAL CHEMISTRY

#### **Theory : 60 Hours (04 Credits)**

#### **SECTION A**

#### 1. Quantum chemistry II

#### (20 Hours)

Qualitative treatment of hydrogen atom and hydrogen – like ions; setting up of Schrodinger equation in spherical polar co-ordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus. Setting up of Schrodinger equation for many-electron atoms (He, Li) Need for approximation methods. Statement of variation theorem and application to simple systems (Particle in a box, harmonic oscillator, hydrogen atom)

Chemical Bonding: Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of  $H_2^+$ . Bonding and antibonding orbitals, qualitative extension to  $H_2$ , comparison of LCAO-MO and VB treatments of  $H_2$ . (Only wave functions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homo-nuclear and hetero-nuclear diatomic molecules (HF, LiH).

#### 2. Nuclear Chemistry II

Nuclear Fission, discovery, energy released in fission, fission products, neutron emitted in fission, nuclear reactors, classification of reactors, Breeder reactor, nuclear reactors in India, chain Reactions & its control, reprocessing of spent fuels Units of radiation energy, applications of radio-isotopes, radioisotopes as tracers, biological effects of radiation.

#### **SECTION B**

#### 3. Electrochemistry II

Definition of pH, pOH, pKa, and pK $_b$ , Determination of pH using glass electrodes by potentiometric method, Buffer solution, types, buffer action, buffer capacity, mechanics of buffer action, Henderson equation for acidic and basic buffer, amphoteric electrolyte, existence of dipolar ions, isoelectric point, strong electrolytes, Debye Huckel theory of strong electrolytes.

#### (10 Hours)

(12 Hours)

Variation of activity coefficient with concentration, ionic strength, Debye Huckel limiting law.

Energy sources: Primary and Secondary batteries. Acid and Alkaline battery, Ni-Cd cell, solar cells, Construction, working, advantages and CdS solar cell. [Ref. 4, 9, 10, 11]

#### 4. Molecular Spectroscopy II

#### (18 Hours)

Electronic Spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and pre dissociation, calculation of electronic transitions of polyenes using free electron model.

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Armor precession, Chemical shift and low resolution spectra, different scales (Delta and T), Spin –spin coupling and high resolution spectra, interpretation of PMR spectra of organic molecules.

Electron Spin Resonance (ESR) spectroscopy: Principle, hyperfine structure, ESR of simple radicals.

#### **Text Books:**

- 1. J.N. Gurtu, Physical Chemistry Vol-III, A pragati edition.
- 2. N. B. Laxmeshwar, S. M. Malushte, A. S. Mulye, V. N. Kulkarni, Concepts of Physical Chemistry, Chetana Prakashan.
- P. C. Jain, Monika Jain, Engineering Chemistry, 15<sup>th</sup> edition, Dhanpat Rai Publishing Co.

#### **Reference Books:**

- Barnwell, C.N. & McCash, E.M., Fundamentals of Molecular Spectroscopy, 4<sup>th</sup> Ed. Tata McGraw Hill, New Delhi (2006)
- 2. U. N. Dash, Nuclear Chemistry, S. Chand Publication
- H. J. Arnikar, Essentials of Nuclear Chemistry, New Age International Publishers, 4<sup>th</sup> Revised Edition
- 4. Gurdeep Raj, Advanced Physical Chemistry Goel Publication.
- 5. Chandra, A.K., Introductory Quantum Chemistry, Tata McGraw -Hill (2001).
- 6. House., J.E., Fundamentals of Quantum Chemistry, 2<sup>ND</sup> Ed. Elsevier: USA (2004)
- 7. Lowe. J.P. & Peterson., K., Quantum Chemistry, Academic Press (2005)

### SEMESTER VI CHEMISTRY-LAB CORE COURSE: CHC108 PHYSICAL CHEMISTRY

#### Practicals: 60 Hours (02 Credits)

- Conductometric titration of Lead Nitrate against Sodium Sulphate and to determine the solubility of Lead Sulphate. [Ref. 4]
- 2. Using vibrational-rotational spectra of NO and CO molecules; [Ref. 1]
  - a. Assign the rotational lines to various transitions.
  - b. Calculate i) the value of  $B_0$  and  $B_1$ , for R and P branches of spectra.
    - ii) Vibrational frequency and
    - iii) Inter nuclear distance

c. Draw the vibrational-rotational energy levels and show the various transitions of R and P branches.

- 3. To investigate the influence of Ionic strength on the rate constants between Potassium Persulphate and Potassium Iodide. [Ref. 4]
- 4. To determine the dissociation constant of a weak dibasic acid using pH metry. [Ref. 4]
- 5. To study the Kinetics of ethyl acetate by NaOH at two different temperatures and hence determine the energy of activation. [Ref. 4]
- 6. To determine the percentage concentration and strength of sulphuric acid, acetic acid and copper sulphate against 0.1 M NaOH by conductometric titration. [Ref. 3]
- 7. Preparation of aniline hydrochloride and to determine hydrolysis and hydrolysis constant of aniline hydrochloride. [Ref. 4]
- 8. Adsorption of Oxalic acid by charcoal and verifying Freundlich adsorption isotherm. [Ref. 4]
- 9. Verification of Debye-Huckel-Onsager equation to dilute solutions of KCl by conductometric method. [Ref. 4]
- 10. To determine the strength and concentration of a mixture of HCl and H<sub>2</sub>SO<sub>4</sub> against 0.1 M NaOH by potentiometric titration. [Ref. 3]

#### (10 x 6 Hours)

#### Text Book:

1. Systematic experimental Physical Chemistry by W. Rajbhoj, T.K. Chondhekar, Anjali publication.

#### **<u>Reference Books</u>**;

- 1. Practicals in Physical Chemistry a modern approach by P.S. Sindhu, published by Macmillan India Ltd.
- Practical Physical Chemistry by B. Viswanathan, P.S. Raghavan, published by Viva Books Private Ltd.
- 3. Senior Practical Physical chemistry by B.D. Khosla, V.C. Garg, Adarsh Gulati, published by R. Chand and Co.

## SEMESTER VI CORE COURSE: CHC109 (06 Credits: Theory-04, Practicals-02)

#### (INORGANIC CHEMISTRY)

#### Theory: 60 Hours (04 Credits)

#### SECTION A

#### 1. Organometallic chemistry

#### (15 Hours)

(15 Hours)

Definition, nomenclature and classification of organometallic compounds, EAN rule, 18 electron rule.

- (A) Mononuclear metal carbonyls: Preparation, properties, structure and bonding of Ni(CO)<sub>4</sub>, Fe(CO)<sub>5</sub> and Cr(CO)<sub>6</sub> (Orbital diagram not expected)
- (B) Polynuclear metal carbonyl: Preparation and structures of Mn<sub>2</sub>(CO)<sub>10</sub>, Co<sub>2</sub>(CO)<sub>8</sub>
   Fe<sub>2</sub>(CO)<sub>9</sub> and Fe<sub>3</sub>(CO)<sub>12</sub> (Orbital diagram not expected)
- (C) Sandwich compounds like Ferrocene: preparation, properties, reactions, structure and

Bonding(MOT).

(D) Preparation and properties of alkyl and aryls of Li, Al, Hg and Ti.

#### 2. Spectra and Magnetic properties

- A) Effect of Crystal Field Splitting on properties of Octahdral Complexes: Magnetic, Spectral. Measurement of 10 Dq for [Ti(H<sub>2</sub>0)<sub>6</sub>]<sup>+3</sup> Complex.
- B) Determination of ground state term for d<sup>1</sup> to d<sup>10</sup> metal ions
- C) Electronic Spectra of transition Metal Complexes.
   Introduction, Types of Electronic transitions. The d-d transitions (d<sup>1</sup>/d<sup>9</sup> and d<sup>2</sup>/d<sup>8</sup>), Charge transfer transitions and Ligand- Ligand transitions.
   Selection Rules (laporte Orbitals and Spin). Applications: Ligand field strength, Colour of complexes, Cis Trans isomerism and Geometry of complexes.
- D) Types of magnetic behaviour, Methods of determining magnetic susceptibility (Gouy's method); Spin only formula; application of magnetic moment data for 3d – Metal complexes

#### **SECTION B**

#### 3. Reaction Kinetics and Mechanism

A brief outline of thermodynamic stability of metal complexes and factors affecting the stability. Thermodynamic and Kinetic stability, Lability and inertness of octahedral complexes, Taube's classification. Kinetics of octahedral complexes: Electrophilic and Nucleophilic substitution. Mechanism of ligand substitution in octahedral complexes: acid hydrolysis, base hydrolysis and annation reaction. Trans- effect with respect to square planar Platinum complexes.

#### 4. Acid Bases and Non-aqueous Solvents

Bronsted theory, Lux – Flood Solvent systems and Lewis concept of Acids and Bases. Classification and physical properties of solvents, their general characteristics and levelling effect. Reactions in non-aqueous solvents with respect to liquid NH<sub>3</sub>, liquid SO<sub>2</sub> and liquid HF.

#### 5. Symmetry and Term Symbols

Symmetry elements like Centre of symmetry, Rotation axis. Mirror Plane, Rotation Reflection Axis, Identity. Determination of Point group and its application to H<sub>2</sub>O, Ethylene, Trans dichloro ethylene, NH<sub>3</sub>, BCl<sub>3</sub>, [PtCl<sub>4</sub>]<sup>-2</sup>, SiCl<sub>4</sub>, Benzene, SF<sub>6</sub>.

#### Text books:

- 1. J. D. Lee, *Concise Inorganic* Chemistry, 5<sup>th</sup> Edn. Wiley India.
- B. R. Puri, L. R. Sharma and K. C. Kalia, *Principles of Inorganic Chemistry*, 33<sup>rd</sup> Edn.

#### **Reference books:**

 F. Albert Cottton, Geoffrey Wilkinson and Paul L. Gaus, *Basic inorganic chem*. 3<sup>rd</sup> Edn. Wiley India

#### (10 Hours)

#### (8 Hours)

(12 Hours)

- James E. Huheey, Ellen A. Keiter, Richard L.Keiter and Okhil K. Medhi, Inorganic Chemistry, Principles of Structure and Reactivity. 4<sup>th</sup> Edn. Pearsons
- K. V. S. Laxmi Devi, N. C. Patel, S.S. Dhume, A. Venkatachalam, S. P. Turakhia, Chhaya Dixit and R. A. Mirji, College Inorganic Chemistry for T.Y. B. Sc. 21<sup>st</sup> Edn, Himalaya Publishing House.
- **4.** Solid State Chemistry, Third edition By- Lesley E. Smart, Elaine A. Moore, Pub-Taylor and Francis.
- 5. D. E. Shriver, P.W. Atkins and C.H. Langford, Inorganic Chemistry, Oxford.
- **6.** G.D. Tuli, S. K. Basu and R.D. Madan, Advance inorganic chemistry, Satya Prakash, S. Chand Publication.
- 7. F. A. Cotton, Chemical Applications of Group Theory, Wiley India
- **8.** P.K Bhattacharya ,Group Theory and its Chemical Applications Himalaya Publications.

## SEMESTER VI CHEMISTRY- LAB CORE COURSE: CHC109 (INORGANIC CHEMISTRY)

## Practicals: 60 Hours (02 Credits)

## Volumetric Exercises

- 1. Volumetric estimation of Nitrite in the given solution of sodium nitrite using KMnO<sub>4</sub>
- 2. Estimation of Fe(III) by dichromate method in the given solution of ferric alum by using SnCl<sub>2</sub>.
- 3. Preparation of Tetraaminecopper(II) sulphate complex and estimate the amount of copper from Tetraaminecopper(II) sulphate complex by iodometry.
- 4. Preparation of Trisethylenediaminenickel(II) chloride complex and estimate the amount of Ni by EDTA.
- 5. Estimate volumetrically the amount of cobalt in CoCl<sub>2</sub>. H<sub>2</sub>O by EDTA method using hexamine indicator.
- 6. To estimate amount of  $ferrous(Fe^{2+})$  and  $ferric(Fe^{3+})$  ions in the given solution containing ferric chloride and ferrous sulphate by using potassium dichromate.
- 7. To estimate aluminium by back titration using zinc sulphate.
- 8. Estimation of manganese in presence of iron in ferromanganese by EDTA titration.
- Determine the strength in grams per litre of a given AgNO<sub>3</sub> solution being provided N/30 NaCl solution by Mohr's Method.
- 10. Determination of alkalinity of a given mixture of OH<sup>-</sup> and CO<sub>3</sub><sup>-2</sup> using phenolphthalein and methyl orange indicator.

# [Note : Pre-sessions are expected to explain the principle, procedure and calculations of each experiment]

Text book :

 G.H. Jeffery, J. Bassett, J. Mendham, R. C. Denney, Vogel's Textbook of Quantitative Chemical Analysis, 5<sup>th</sup> Edn. ELBS

#### **Reference books :**

1. J. Mendham, R. C. Denney, J.D. Barnes, M. Thomas, B. Sivasankar, Vogel's Textbook of Quantitative Chemical Analysis, 6<sup>th</sup> Edn. Pearson

- 2. S. Ratan, Experiments in Applied Chemistry, 3rd Edn. S.K. Kataria & Sons
- 3. O. P. Pandey, D. N. Bajpai and S. Giri, Practical Chemistry, Revised Edn. S. Chand.

#### SEMESTER VI CORE COURSE: CHC110 (06 Credits: Theory-04, Practicals-02)

#### (ORGANIC CHEMISTRY)

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#### **Theory: 60 Hours (04 Credits)**

#### SECTION A

#### **1. Name Reactions and Rearrangements**

#### (18 hours)

Reaction and mechanism of the following: Benzoin, Aldol, Knoevanagel, Wittig and Darzens Glycidic ester. Rearrangement with mechanism: Beckmann, Wolff Rearrangement and Hofmann. Only Reaction and applications (2) of the following: Baeyer Villiger, Appel, Diekmann and Stobbe. Rearrangements: Schmidt, Claisen, Favorskii ,Curtius. Comparison of Clemmensen reduction and Wolff Kishner reduction.

#### 2. Chemistry of Enolates

Definition of enolate ion, acidity of carbonyl compounds, pka values, generation of enolate ion, role of bases in enolate ion formation, alkylation of carbonyl compounds with reference to cyclohexanone, acetone, ethylacetoacetate, malonic ester. Claisen condensation for preparation of ethylacetoacetate (reaction and mechanism). Keto-enol tautomerism of ethylacetoacetate. Malonic ester synthesis of carboxylic acids, ethylacetoacetate synthesis of ketones. Alkylation of 1,3-dithianes. Alkylation via enamine synthesis. Michael addition reaction.

#### 3. Photochemistry

Jablonski diagram, fluorescence, phosphorescence, intersystem crossing and vibrational relaxation. Norrish Type I and Type II cleavage reactions of ketones. Paterno Buchi and Barton reaction.

#### **SECTION B**

#### 4. Terpenes

Structure elucidation of Citral,  $\alpha$ -Terpineol,  $\alpha$ -Pinene and Camphor. Synthesis of Methylheptenone, Terebic acid and terpenylic acid. Synthesis of Citral from Methylheptenone. Synthesis of  $\alpha$  –Terpineol from p-toluic acid. Synthesis of Norpinic acid, camphoric acid, camphoronic acid. Commercial synthesis of camphor.

#### (8 Hours)

#### (4 Hours)

(16 Hours)

#### 5. Carbohydrates

#### (6 Hours)

(8 hours)

Open chain reactions of Glucose, Ruff degradation, determination of ring size of Glucose (pyranose and furanose using methylation method).

Open chain reactions of sucrose, inversion of canesugar, Evidence of presence of glucose and fructose unit in sucrose. Determination of ring size of Sucrose. (using methylation method).

#### 6. Stereochemistry

Stereospecific and stereoselective reactions. Addition of bromine to 3-Hexene with mechanism. Addition of hydrogen halides to alkenes: Markownikoff's and anti-Markownikoff's addition rule. Substitution reactions: SN1, SN2, SNi reactions with mechanisms. Elimination reactions: E1, E2, E1cb reactions with mechanism.

#### Text books :

- 1. I.L.Finar, Organic Chemistry Vols I and II, Orient Longman
- 2. Morrison and Boyd, Organic Chemistry; 6th Edn. Prentice Hall India
- 3. J. March, Advanced Organic Chemistry: Reaction, Mechanism and Structure, Wiley, 2010, 4th Ed.
- I.L. Finar, Stereochemistry and Chemistry of Natural products, ELBS, Longmans, 1963, Vol. 2, 3rd Ed.

5. P.S. Kalsi, Spectroscopy of Organic compounds, New Age International Pub. Ltd. & Wiley Eastern Ltd., Second edition, 1995.

#### **Reference books**

- 1. Francis Carey, Organic Chemistry, 10<sup>th</sup> Edition.
- 2. Paula Yurkanis Bruice, Organic Chemistry; 3rd Edn. Pearson Education Asia
- 3. Silverstein, Bassler and Morill, Spectrometric Identification of Organic Compounds;
- P Sykes, A guidebook to mechanisms in organic chemistry, 6th Ed., Pearson Edu., 1996.
- J. Clayden, N. Greeves, S. Warren & Wothers, Organic Chemistry, Oxford University Press, 2012, 2nd Ed.
- 6. E.S. Gould et al., Mechanism and structure in Organic Chemistry, 1965
- 7. F. A. Carey, Organic Chemistry, 2000, 4th Ed.
- 8. S.H. Pine, Organic Chemistry, McGraw-Hill International Edn. 2010, 5thEd.

- F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Vol. I & II. Plenum Press, 1977.
- D. Nasipuri, Stereochemistry of Organic compounds Principles and Application, Wiley Eastern Limited, 2013, 4th Ed. Kent, [England]: New Academic Science Limited, 2013.
- E.L. Eliel, Stereochemistry of carbon compounds, Tata MacGraw Hill Publishing Company Ltd. (1990)
- 12. V.M. Potapov, Stereochemistry, MIR Publishers, Moscow, 1979
- 13. Organic Photochemistry- A Visual Approach, J Kopecky, VCH Pub., 1992.
- Applications of Absorption Spectroscopy of Organic compounds, J. R. Dyer, Prentice Hall of India, 1987.
- V.M. Parikh, Absorption spectroscopy of organic Molecules, Addison Wesley Longman Publishing Co., 1974.
- D.H Williams & I. Fleming, Spectroscopic methods in organic chemistry, 6th Ed., Tata Mcgraw Hill Education, 2011.
- William Kemp, Organic spectroscopy, 3<sup>rd</sup> Ed., Palgrave Macmillan, 1991.
- R. O. C. Norman and J. M. Coxon, Principles of Organic Syntheses, 3rd Ed., CRC Press Inc, 1993.
- R. Bruckner, Advanced Organic Chemistry Reaction Mechanisms, San Diego, CA: Harcourt /Academic Press, San Diego, 2002.
- M. B. Smith, Organic Synthesis, McGraw HILL International Edition, New York, 1994.
- W. Caruthers, Modern Methods of Organic Synthesis, 4th Ed., Cambridge University Press, 2004.
- 22. Heterocyclic Chemistry, J A Joule and G F Smith, ELBS, Advances in Heterocyclic Chemistry, Edited by A R Katritzky etal, Vol. 1 to 50, Academic P

## SEMESTER VI CHEMISTRY LAB CORE COURSE: CHC110 (06 Credits: Theory-04, Practicals-02) (ORGANIC CHEMISTRY)

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#### Practicals: 60 hours (02 Credits)

#### 1. Preparation of Derivatives (Any 4)

- i) Oxime derivative of Benzophenone.
- ii) Acetyl derivative of Salicylic acid
- iii) Osazone of Fructose
- iv) Aldol derivative (using benzaldehyde and acetone to give dibenzalpropanone)
- v) Benzoyl derivative of p-nitroaniline

\*Demonstration of Knoevanagel condensation between Salicylaldehyde and

ethylacetoacetate.

#### **Ref. 1 to 7**

#### 2. Binary mixture separation and analysis (Microscale)

#### (Any 10 Mixtures to be analysed)

Water insoluble –water insoluble (4 mixtures)

(Acid-Base, Acid-Phenol, Base-Neutral, Acid-Neutral, Phenol-Base, Phenol-Neutral.

Water soluble –water insoluble (2 mixtures)

(Acid-Acid, Acid-Neutral, Neutral-Neutral).

Liquid-Liquid (2 mixtures)

Solid-liquid mixture. (2 mixtures)

#### Text books :

- 1. A.I. Vogel, A.R. Tatchell, B. S. Furniss, A.J. Hannaford, *Vogel's Textbook* of *Practical Organic Chemistry*, 5th Ed., Prentice Hall; 2011.
- 2. Practical organic chemistry, F G Mann and B C Saunders, Orient Longman, 4th ed.
- 3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*, Universities Press.

#### **Reference books :**

**1.** D. Pasto, C. Johnson and M. Miller, *Experiments and Techniques in Organic Chemistry*, 1st Ed., Prentice Hall, 1991.

2. L.F. Fieser, K.L. Williamson "Organic Experiments" 7th edition D. C. Heath, 1992.

3.K.L. Williamson, K.M. Masters, Macroscale and Microscale Organic

Experiments, 6th Edition, Cengage Learning, 2010

4.R.K. Bansal, *Laboratory Manual in Organic Chemistry*, New Age International, 5th Edition, 2016.

## SEMESTER VI DISCIPLINE SPECIFIC ELECTIVE: CHD103

#### (04Credits: Theory- 04)

#### (SELECTED INSTRUMENTATION IN CHEMISTRY)

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#### **Theory: 60 Hours (04 Credits)**

#### SECTION A

#### 1. Introduction:

Overview of instruments in chemical analysis, Basic components of instruments for analysis: Signal generators, detectors (input transducers) Signal processors, read out devices, circuits & electrical devices in the instruments, advantages of instruments interfaced with computers.

#### 2. Chromatographic techniques:

Classification of chromatography methods.

Gas chromatography: Basic principles of GSC and GLC. Terms involved: Distribution equilibria, rate of travel, retention time, retention volume, relative retention, Height Equivalent to a Theoretical Plate(HETP), Van Deemter equation.

Instrumentation: carrier gas, column, injections systems, explanations of factors affecting separation, thermal conductivity and flame ionization detectors. Qualitative and Quantitative analysis: internal standards, determination of peak area.

HPLC: Instrumentation, description of pumps, detector choice (UV absorption and refractive index detectors), columns, injection system, packing materials, applications. Introduction to hyphenated techniques: Basic principles of GC-MS and LC-MS.

(Numerical problems are to be solved)

#### 3. Mass spectrometry:

Introduction, theory, making the gaseous molecule into an ion (electron impact, chemical ionization), making liquids and solids into ions (electrospray, electrical discharge), separation of ions on basis of mass to charge ratio.

Instrumentation: schematic diagram of single and double focussing. Advantages of Quadrupole Mass Spectrometer, sample introduction, sample purity, spectrum resolution. Applications of mass spectrometry in structure elucidation. Peak matching.

#### (8 Hours)

## (12 Hours)

(4 Hours)

#### 4. X-ray diffraction methods:

Introduction to X-ray absorption and emission methods, Bragg's law, Diffraction of X-rays, production and detection of X-rays, sample preparation, identification of powder diffraction patterns of ZnO, NiO and MgAl<sub>2</sub>O<sub>4</sub>.

#### **SECTION B**

#### 5. UV-Visible Spectroscopy:

Interaction of electromagnetic radiation with matter, Quantitative calculations- Beer's and Lambert's law, derivation of Beer-Lambert's law, deviations from Beer's law.

Principles of instrumentation: Sources, monochromators, cells.

Types of instruments: Photoelectric colorimeters and Spectrophotometers: Single & Double beam; comparison between colorimeter and spectrophotometer; applications: qualitative control of purity, quantative analysis; identification of structural groups in a molcule; study of co-ordination compound, cis-trans isomerism; chemical kinetics. Photometric titrations *(numerical problems are expected to be solved)* 

#### 6. Atomic spectrometric methods:

Atomic absorption Spectroscopy: Introduction, principle, instrumentation, applications, limitations.

Flame photometry and introduction, principle, instrumentation, applications, limitations. Differences between flame photometry and atomic absorption spectroscopy.

Fluorimetry: principles of fluorescence, chemical structure and fluorescence. Relationship between concentration & fluorescence intensity, instrumentation & applications. *(numerical problems are expected to be solved)* 

#### 7. Analysis of drug in solid state:

Concepts of particle size, size distribution shown as cumulative undersize curve.

Thermal methods of analysis: Basic principles of differential thermal analysis(DTA) and Differential Scanning Calorimetry(DSC), Differential Thermal Analysis - apparatus and methodology, factors affecting DTA results, quantitative DTA, interpretation of results. Applications to detect polymorphism and pseudopolymorphism in pharmaceuticals by DSC or DTA.

#### (6 Hours)

(10 Hours)

#### (14 Hours)

#### (6 Hours)

#### Text books :

1. B. K. Sharma. Instrumental Methods of Chemical Analysis: Goel Publishing House, Meerut

2. K.Raghuraman, D. V. Prabhu, C. S. Prabhu and P. A.Sathe, Basic principles in Analytical Chemistry, 5<sup>th</sup> edition, Shet Publications pvt.ltd.

#### **Reference books:**

- G. Chatwal and S. Anand, Instrumental Methods of Chemical Analysis, 5<sup>th</sup> edition (reprint 2003), Himalaya publication.
- 2. Willard, Meritt and Dean. Instrumental Methods of Analysis.
- 3. Skoog and Leary, Principles of Instrumental analysis, Saunders College Publication.