# St. Xavier's College (Autonomous), Mumbai



Syllabus of the courses offered by the Department of Chemistry (2015-16)



# St. Xavier's College – Autonomous Mumbai

# Syllabus for 1st Semester Course in CHEMISTRY(June 2014 onwards)

Contents: Theory Syllabus for Courses: S.CHE.1.01 –CONCEPTS OF PHYSICAL AND ANALYTICAL CHEMISTRY I S.CHE.1.02 - FUNDAMENTALS OF INORGANIC AND ORGANIC CHEMISTRY I PRACTICAL COURSE SYLLABUS FOR S.CHE 1 PR

# SYLLABUS UNDER AUTONOMY CHEMISTRY

# SEMESTER I COURSE: S.CHE.1.01 CONCEPTS OF PHYSICAL AND ANALYTICAL CHEMISTRY I [45 LECTURES]

#### **LEARNING OBJECTIVES**

- 1. To understand mole concept, concentration calculations and stoichiometric relations.
- 2. To apply inter conversions to relate various concentration units.
- 3. To differentiate between primary and secondary standards.
- 4. To understand the importance of accuracy, precision, errors and its sources, presentation of experimental data and significant figures.
- 5. To understand the behaviour of fluids and study the physical phenomena involved.
- 6. To understand the statistical methods of representing experimental data.
- 7. To understand the kinetics of various order reactions and apply these concepts to various categories of catalysed reactions.

# Unit I: Introduction to Analytical Chemistry and its interdisciplinary nature (15 L)

#### 1.1: Chemical Calculations and Stoichiometry

- **1.1.1:**Moleconcept, determination of molecular massby gram molecular volume relationship for chemicalreactions, problemsbased on mole concept.
- **1.1.2:**Methods of expressing concentration of solutions: molarity, normality, molality, mole fraction, formality, dilution of solutions, inter-conversion between different concentration units, conceptof milliequivalents, millimoles, ppm and ppb.
- **1.1.3:** Analysis of Commercial Samples: Calculation of concentration of commercial samples of acids and bases like HCl, H<sub>2</sub>SO<sub>4</sub>, acetic acid and ammonia.
- **1.1.4:** Gravimetric and Volumetric analysis: use of digital balance, calibration of glassware, pipette, burette and volumetric flask, primary and secondary standards.
- **1.1.5:**Importance of accuracy, precision and sources of error in analyticalmeasurements, presentation of experimental data and results from the point of view of significant figures.

# **Unit II: Study of Fluids**

(15 L)

#### 2.1:Behaviour of Real Gases

(9 L)

**2.1.1**: Recapitulation of ideal behaviour of gases, deviations from ideal gas behaviour, compressibility factor - Z and its variation with pressure for different gases. Causes of deviation from ideal behaviour.

- **2.1.2:** Van der Waal's equation of state, its derivation and application in explaining real gas behaviour(Mention of other equations of state: Berthelot, Dietrici).
- **2.1.3:** Isotherms of real gases and their comparison with Van der Waal's isotherms, continuity of states, critical state, experimental determination of Pc, Tc and Vc, critical constant of gas in terms of Van der Waal's constant.

#### 2.2: Physical properties of Liquids

(6 L)

- **2.2.1:** Measurable physical properties of liquid such as vapour pressure, surface tension and viscosity.
- **2.2.2:** Experimental determination of vapour pressure, surface tension and coefficient of viscosity (one method of each), effect of addition of various solutes on surface tension and viscosity.
- **2.2.3:**Temperature variation of viscosity of liquids and comparison with that of gases.

#### **Unit III: Kinetics and Catalysis**

(15 L)

#### 3.1: Kinetics (10 L)

- **3.1.1:** Graphical representation of equations:Co-relation between mathematical functions and shapes of the graph, rules for drawing graph co-ordinates etc., equation of straight line, slope and intercept, plotting the graph from the data of chemical properties, determination of equation of line of best fit (method of averages and least squares) for y = mx only and problems.
- **3.1.2:** Recapitulation of basic concepts: Rate law, specific rate constant, comparison between order and molecularity with examples, integrated rate equations for zero and firstorder reactions and their half life (no derivations), numerical problems expected.
- **3.1.3:** Second order reaction: Derivation of integrated rate equation (for equal and unequal concentration of reactants), characteristics of second order reactions with suitable examples, effectof temperature on rate of reaction (no derivation expected for Arrhenius equation).

#### 3.2: Catalysis (5 L)

- **3.2.1:**Catalyst and catalysis, positive and negative catalysis, type of catalysis, characteristics of catalytic reactions, promoters, catalytic poisoning, autocatalysis.
- **3.2.2:** Activation energy and catalysis, theories of catalysis, active centre on catalyst surface, adsorption theory and catalytic activity (theoretical aspect only).
- **3.2.3:**Acid Base catalysis (theoretical aspect only) and its applications in industry.
- **3.2.4:**Enzyme catalysis, mechanism of enzyme catalysis, characteristics of enzyme catalysis, effect of temperature on enzyme catalysis (**qualitative approach only**), applications.

#### **REFERENCES:**

- 1. Principles of Physical Chemistry,4th edition by S.H. Marron and C.F.Pruton.
- 2. Textbook of Physical Chemistry, Samuel Glasstone.
- 3. Physical Chemistry, Ira Levine, 5th Edition, 2002 Tata McGraw Hill Publishing Co. Ltd. [Chapter 4,14].
- 4. Physical Chemistry, G.M. Barrow, 6th Edition, Tata McGraw Hill Publishing Co. Ltd. New Delhi.
- 5. Physical Chemistry 9th Ed., Atkins, P. W. & Paula, J. de Atkins Oxford UniversityPress2011.
- 6. University Chemistry, Bruce Mahan.
- 7. Textbook of Physical Chemistry, Sharma and Puri.
- 8. Fundamentals of analytical chemistry, 8<sup>th</sup> edition, Skoog, West, Holler and Crouch.
- 9. Physical Chemistry, 3rd Ed., Ball, D. W. Cengage India.2012.
- 10. Physical Chemistry 4th Ed., Castellan, G. W. Narosa 2004.
- 11. Chemical Kinetics, J. LaidlerK. Pearson Education: New Delhi 2004.
- 12. Rogers, D. W. Concise Physical Chemistry Wiley 2010.

CIA I: Short answer questions and cross-word

20 MARKS

CIA II: MCQ

20 MARKS

# **Template of Question Paper**

# CONCEPTS OF PHYSICAL AND ANALYTICAL CHEMISTRY I COURSE: S.CHE.1.01

#### **OBJECTIVES**

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL MARKS
I	4	4	12	20
II	6	8	6	20
III	3	7	10	20
TOTAL MARKS PER OBJECTIVE	13	19	28	60
% WEIGHTAGE	22	32	46	100

# END SEMESTER PAPER PATTERN:

Total Marks: 60 Maximum Time: 2 hours

Total number of questions: 3 [all compulsory] of 20 marks each

1 question per unit.

Question set out of 30 marks [50% internal choice]

Sub questions will not exceed 5 marks.

# SEMESTER I COURSE: S.CHE.1.02 FUNDAMENTALS OF INORGANIC AND ORGANIC CHEMISTRY I [45 LECTURES]

#### **LEARNING OBJECTIVES**

- 1. To reinforce the basics of Inorganic Chemistry with special reference to atomic structure, periodic table and periodicity of properties.
- 2. To study the chemistry of the 's' block elements with emphasis on physical and chemical properties.
- 3. To understand the anomalous behaviour of Lithium and Berylium and the diagonal relationship.
- **4.** To study the trends of properties of the 'p' block elements.
- **5.** To understand Group 18 elements.
- **6.** To understand the principles and theory in Qualitative Analysis of a mixture of radicals especially when they interfere with each other in the detection.
- **7.** To correctly name an organic compound using IUPAC nomenclature and to accurately represent an organic compound given a IUPAC name.
- **8.** To introduce mechanism of organic reactions and to learn to classify reaction types and intermediates.
- **9.** To investigate nucleophilic substitution as well as elimination reactions in detail including a comparative analysis.

#### UNIT I: Fundamentals of Inorganic Chemistry and Chemistry of s-block elements (15L)

#### 1.1:Atomic Structure (3L

Bohr's theory of Hydrogen atom, wave theory, Heisenberg's Uncertainty Principle, orbitals (shapes of s,p and d orbitals), quantum numbers.

#### 1.2: Periodic Table and Periodicity of properties

(3L)

Arrangement of elements in the long form of the periodic table, correlation of classification of elements into s, p, d and f-block on the basis of electronic configuration, Pauli's Exclusion Principle, Aufbau Principle and Hund's Rule of maximum multiplicity, anomalies in electronic configuration.

#### 1.3: Periodic Properties

(4L)

- **1.3.1:** Atomic and ionic radii, ionization energy, electron affinity, effective nuclear charge and calculations using Slater's Rule, electronegativity and its determination using Mulliken's and Pauling's method (numerical problems expected), metallic and non-metallic character, oxidation states, melting / boiling points, colour, magnetic properties, polarizability.
- **1.3.2:** Trends in the periodic table and applications in predicting and explaining chemical behaviour.

#### 1.4: Chemistry of 's' block (Groups 1 and 2)

(5L)

- **1.4.1:** Position of elements in the periodic table, electronic configuration, trends in the properties with respect to family relationship, physical and chemical properties, ionization potential (charge to size ratio), electronegativity, polarizing power, oxidation state, hydration energy of ions
- **1.4.2:** Anamolous behaviour of Li and Be and diagonal relationship.

**1.4.3:** General methods of preparation of organolithium and organomagnesium compounds with applications.

# UNIT II: Chemistry of 'p' block and Group 18 elements and theory of Qualitative Analysis (15L)

#### 2.1: Chemistry of 'p' block elements

(4L)

Position of elements in the periodic table, electronic configuration, trends in periodic properties with respect to family relationship, physical and chemical properties, ionization potential (charge to size ratio), electronegativity, oxidation state and metallic character.

#### 2.2: Chemistry of Group 18

(3L)

History, peculiar properties of Helium, clathrate compounds, preparation of Xenon compounds.

#### 2.3: Principles involved in Qualitative Analysis

(8L)

- **2.3.1:** Use of borax, sodium carbonate, cobalt nitrate, hydrogen sulphide and ammonium chloride in qualitative analysis.
- **2.3.2:** Detection of the following acid radicals in presence of each other: carbonate, sulphite, chloride, bromide, iodide, nitrite and nitrate.

#### **UNIT III: Fundamentals of Organic Chemistry**

(15L)

- **3.1:** IUPAC nomenclature: ALIPHATIC system only (including cyclic systems) with multiple functional groups. (2L)
- **3.2:** Geometry and structure of sp<sup>3</sup>, sp<sup>2</sup> and sp hybridized carbon, nitrogen and oxygen atoms and some common functional groups eg. carbonyl and cyano.

#### 3.3: Applications of electronic factors

(4L)

- **3.3.1**: Impact of inductive effect on  $pK_a$  and  $pK_b$ .
- **3.3.2:** Resonance in organic compounds.
- **3.3.3:** Hyperconjugation and effect on stability of carbocation and carbon radicals.

#### 3.4: Reaction Mechanism

(7L)

- **3.4.1:** Introduction including bond fission, classification of reactions, reagents and intermediates
- **3.4.2:** Structure and stability of carbocations, carbanions and carbon radicals.
- **3.4.3:** Mechanism of nucleophilic substitution, SN<sub>1</sub>, SN<sub>2</sub> and SN<sub>i</sub>. Effect of substrate, nucleophile, leaving group and solvent on rate of reaction.
- **3.4.4:** Elimination Reactions  $E_1$  and  $E_2$ .
- **3.4.5:** Rearrangements of intermediates [hydride and methyl shift].
- **3.4.6:** Elimination v/s Substitution, emphasis on factors that influence substitution / elimination.

#### **REFERENCES:**

- 1. Organic Chemistry, R.T. Morrison and R.N. Boyd, 6<sup>th</sup> Edition, Pearson Education.
- 2. Organic Chemistry, T.W.G. Solomon and C.B. Fryhle, 8<sup>th</sup> Edition, John Wiley & Sons.

- 3. Organic Chemistry, Paula Y. Bruice, Pearson Education, 2008.
- 4. Organic Chemistry, John McMurray
- 5. Organic Chemistry, L.G. Wade Jr.,
- 6. Concise Inorganic Chemistry, J.D. Lee, 5<sup>th</sup> edition, Oxford Press.

Advanced Inorganic Chemistry, Volume I, S.Prakash, G.D. Tuli, S.K.Basu, R.D.Madan.

- 7. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, 3rd edition, 1977.
- 8. Inorganic Chemistry, James E. Huheey, 3rd edition, Harper & Row Publishers, Asia, Pte Ltd., 1983.
- 9. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford, 3rd edition, Oxford University Press, 1999.
- 10. Theoretical Inorganic Chemistry, C. M. Day & J. Selbin, Affiliated East West Press Pvt. Ltd., 1985.
- 11. Advanced Inorganic Chemistry, Volume I and II, Bahl, Tuli and Anand.

CIA I: Objective and short answer questions

20 MARKS

CIA II: MCQ

20 MARKS

## **Template of Question Paper**

#### FUNDAMENTALS OF INORGANIC AND ORGANIC CHEMISTRY I COURSE:S.CHE.1.02

#### **OBJECTIVES**

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL MARKS
I	10	06	04	20
II	10	06	04	20
III	04	08	08	20
TOTAL MARKS PER OBJECTIVE	24	20	16	60
% WEIGHTAGE	40	33	27	100

#### **END SEMESTER PAPER PATTERN:**

Total Marks: 60 Maximum Time: 2 hours

Total number of questions: 3 [all compulsory] of 20 marks each

1 question per unit.

Question set out of 26-28 marks with internal choice.

**Sub questions of 2-3 marks.** 

#### PRACTICAL CHEMISTRY

Course No. S.CHE.1.PR

#### **LEARNING OBJECTIVES:**

- 1. To learn to perform experiments that have specific aims with correct techniques.
- 2. To develop skills of observation, recording and analyzing data.
- 3. To learn to present the experimental work in a systematic manner.

#### **SEMESTER I: COURSE 1**

Volumetric Estimations Chemical Kinetics

#### **SEMESTER I: COURSE 2**

Organic Purification Gravimetric Estimation

#### **COURSE 1:**

#### **VOLUMETRIC ESTIMATIONS:**

Determination of percentage composition of a mixture of  $Na_2CO_3 + NaHCO_3$ . Determination of percentage composition of a mixture of Oxalic acid + Potassium oxalate. Estimation of  $Fe^{2^+}$  versus  $K_2Cr_2O_7$  using an internal indicator (diphenylamine).

#### **CHEMICAL KINETICS:**

- 1. To investigate the hydrolysis of methyl acetate in HCl and identify the rate constant graphically as well as by calculations.
- 2. To identify the relative strength of HCl and H<sub>2</sub>SO<sub>4</sub> using hydrolysis of methyl acetate.

#### **COURSE 2:**

#### **ORGANIC PURIFICATION:**

- 1. Organic compounds to be purified by crystallization using water and aqueous alcohol as solvent system, purity to be confirmed by melting point and the yield obtained to be calculated.
- 2. Determination of mixed melting point also to be included.

#### **GRAVIMETRIC ESTIMATION:**

- 1. To study the effect of heat on the following mixtures:
  - a) NH<sub>4</sub>Cl + BaSO<sub>4</sub> and b) Na<sub>2</sub>CO<sub>3</sub> + NaHCO<sub>3</sub> and to calculate the percentage composition of the mixture.
- 2. To determine the water of crystallization of hydrated salts

#### **❖ CIA AND END SEMESTER PRACTICAL EXAMINATION**

**COURSE 1:** Volumetric Estimations + Organic Purification **COURSE 2:** Chemical Kinetics + Gravimetric Estimation

**Journal:** 5 marks per course.

**CIA:** 15 marks per course.

**Duration:** 3 periods to be conducted during regular practicals by the faculty-in-charge CIA for each course will be an exercise to test a practical skill (Qualitative and Quantitative).

**End Semester Examination:** 30 marks per course. This includes a 5 mark written test based on the theory behind all the experiments conducted per course.

**Duration:** 3 hours. Students are to perform two experiments (one per course).

**Batch Size:** Maximum 20 students per batch.

\*

\*



# St. Xavier's College – Autonomous Mumbai

# Syllabus for 2<sup>nd</sup> Semester Course in CHEMISTRY(June 2014 onwards)

**Contents: Theory Syllabus for Courses:** 

S.CHE.2.01 –CONCEPTS OF PHYSICAL AND ANALYTICAL CHEMISTRY II S.CHE.2.02 - FUNDAMENTALS OF INORGANIC AND ORGANIC CHEMISTRY II

PRACTICAL COURSE SYLLABUS FOR S.CHE 2 PR

# SYLLABUS UNDER AUTONOMY CHEMISTRY

SEMESTER II COURSE: S.CHE.2.01

CONCEPTS OF PHYSICAL AND ANALYTICAL CHEMISTRY II [45 LECTURES]

#### **LEARNING OBJECTIVES**

- 1. To study and understand the tenets of thermodynamics pertaining to First and Second Laws of thermodynamics.
- 2. To understand operation of Carnot cycle in order to determine thermodynamic efficiency.
- 3. Significance and mathematical definition of entropy.
- 4. To understand limitation of Second Law/ Necessity to introduce work functions A and G.
- 5. To correlate free energy change and spontaneity of a process.
- 6. To understand and be able to elucidate the difference between molecular and atomic spectra and understand various types of spectroscopy.
- 7. To understand the basic concepts involved in qualitative analysis and solve the numerical problems based on these concepts.
- 8. To understand the fundamentals involved in various titrimetric analysis.

#### **Unit I: Chemical Thermodynamics**

(15 L)

- **1.1.1:** Recapitulation of some important mathematical concepts: derivatives, rules of differentiation and partial differentiation, algebraic, logarithmic and exponential functions. Integration; rules of integration, algebraic and exponential functions. (*Self Study*)
- **1.1.2:** Intensive and extensive properties, state and path functions, isolated, closed and open systems, zeroth law of thermodynamics (definition only).

- **1.1.3:** First Law of thermodynamics: Definition, relation and comparison between heat capacities, calculations of q, w, E and H for reversible, irreversible and free expansion of ideal gases under isothermal and adiabatic conditions, limitations of first law and need for introducing new functions. (numerical problems expected)
- **1.1.4:** Second Law of thermodynamics: Carnot cycle, mechanical efficiency, entropy changes for system and surroundings for reversible and irreversible processes, entropy changes for an ideal gas in isothermal, isobaric and isochoric processes, entropy changes in chemical reactions, entropy changes accompanying state change, physical significance of entropy, need for introducing new functions. (numerical problems expected)
- **1.1.5:** Free Energy Functions: Gibbs and Helmholtz energy; variation of *G* and *A* with *P*, *V* and *T*; Gibbs energy change and spontaneity, exergonic and endergonic reactions, Gibbs-Helmholtz equation, thermodynamic equation of state. (numerical problems expected)

# **Unit II: Introduction to Spectroscopy**

(15 L)

- **2.1.1:** Physical quantities and their dimensions: International system of units, derived units, subsidiary units, prefixes for S.I. units, some important conversion factors.
- **2.1.2:** Interaction of low energy radiation with matter: Electromagnetic spectrum, quantisation of energy, absorption of radiation, absorption process, absorbance, transmittance, Beer's law, absorption spectrum, atomic absorption, molecular absorption, limitations of Beer's Law, Beer Lambert's Law and its applications.
- **2.1.3:** Emission of electromagnetic radiation: Emission spectra, line spectra, band spectra, continuous spectra, effect of concentration on line and band spectrum, emission by fluorescence and phosphorescence (introduction only), electronic, vibrational and rotational energy levels and transitions in atoms and molecules.
- **2.1.4:** Electronic Spectra and Molecular Structure: Kinds of transitions, significance and applications of various types of spectroscopies (qualitative discussion only).

#### **Unit III: Analytical Chemistry**

(15 L)

#### 3.1: Principles of Qualitative Analysis

(9 L)

- **3.1.1:** Buffer solutions: types of buffers, derivation of Henderson–Hesselbelch equation and its applications; buffer capacity, buffer range, buffer action and applications of buffers in analytical chemistry (numerical problems expected).
- **3.1.2:** Solubility product, factors affecting precipitation equilibria (solubility product) in qualitative analysis: common ion effect, pH, complexation, diverse ion effect, oxidation states (numerical problems expected).

#### 3.2: Volumetric Analysis

(6 L)

#### 3.2.1: Classification of volumetric analysis (basic concepts only)

(1 L)

#### 3.2.2: Acid base (neutralisation) titrations:

(1 L)

Theory of indicators, theory of acid base indicators, mixed and universal indicators, explaination of the shapes of neutralisation curves for strong acid - strong base, weak acid - strong base, weak base - strong acid, weak acid - weak base, choice of indicators (numerical problems expected).

#### 3.2.3: Oxidation-Reduction Titration:

(1 L)

Principle and only theoretical discussion (using suitable examples), detection of end points, numerical problems.

# **3.2.4: Complexometric Titration:**

(1 L)

Principle (using suitable examples), standardisation, detection of end point.

## 3.2.5: Iodometry and Iodimetry:

(1 L)

General discussion, detection of end point, difference between iodometry and iodimetry.

# **3.2.6: Precipitation Titration:**

(1 L)

Principle and only theoretical discussion (using suitable examples), detection of end point.

#### **REFERENCES:**

- 1. Mathematical preparation for physical Chemistry By F. Daniel, Mc. Graw Hill publication.
- 2. University General Chemistry. By C.N. R. Rao Mc. Millan Publication.
- 3. Principles of Physical Chemistry. By Maron and Pruton 4th Ed. Oxford and IBH publication.
- 4. Physical Chemistry. By G.M. Barrow.
- 6. Peter, A. & Paula, J. de. *Physical Chemistry 9th Ed.*, Oxford University Press 2011.
- 7. Castellan, G. W. *Physical Chemistry 4th Ed.*, Narosa 2004.
- 8. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.*, Prentice-Hall 2012.
- 9. McQuarrie, D. A. & Simon, J. D. *Molecular Thermodynamics* Viva Books Pvt. Ltd.: New Delhi 2004.
- 10. Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. *Commonly Asked Questions in Thermodynamics*. CRC Press: NY 2011.Page 19 of 80
- 11. Levine, I.N. Physical Chemistry 6th Ed., Tata Mc Graw Hill 2010.
- 12. Metz, C.R. 2000 solved problems in chemistry, Schaum Series 2006.

CIA I: Objective and short answer questions 20 MARKS

CIA II: MCQ 20 MARKS

#### **Template of Question Paper**

# CONCEPTS OF PHYSICAL AND ANALYTICAL CHEMISTRY II COURSE: S.CHE.2.01 OBJECTIVES

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL MARKS
I	4	4	12	20
II	6	8	6	20
III	3	7	10	20
TOTAL MARKS PER	13	19	28	60
OBJECTIVE				
% WEIGHTAGE	22	32	46	100

#### **END SEMESTER PAPER PATTERN:**

Total Marks: 60 Maximum Time: 2 hours

Total number of questions: 3 [all compulsory] of 20 marks each 1 question per unit.

Question set out of 26-28 marks with internal choice.

Sub questions of 2-3 marks.

SEMESTER II COURSE: S.CHE.2.02

#### FUNDAMENTALS OF INORGANIC AND ORGANIC CHEMISTRY II [45 LECTURES]

#### **LEARNING OBJECTIVES:**

- 1. To understand some characteristic properties of elements of groups 13 to 17.
- 2. To study the chemistry of representative elements of groups 13 [aluminium] and 14 [silicon].
- 3. To understand some properties of a few selected compounds of groups 15,16 and 17.
- 4. To introduce manufacturing processes of bulk chemicals [ammonia and sulphuric acid].
- 5. To understand the concept of isomerism, and represent the structures of organic compounds
- 6. To study properties of unsaturated hydrocarbons.
- 7. To study the reactivity of various aliphatic organic compounds and their interconversions in 5-6 steps.

# UNIT I: CHEMISTRY OF p-BLOCK ELEMENTS

(15 L)

1.1: Group 13 (3 L)

- 1.1.1: Structures of electron-deficient compounds with reference to boron hydrides, inert pair effect.
- 1.1.2: Chemistry of Aluminium compounds halides, oxides and alkyls.

# 1.2: Group 14 (3L)

- 1.2.1: Catenation and allotropy with special reference to carbon.
- 1.2.2: Chemistry of silicon, preparation and uses of silicones.

## 1.3: Groups 15 and 16

(6L)

- 1.3.1: Physical properties of hydrides of elements of groups 15 and 16 with respect to hydrogen bonding.
- 1.3.2: Manufacture of bulk chemicals ammonia by Haber's process and sulphuric acid by Contact process [principles, reactions and flow chart expected].

1.4: Group 17 (3L)

1.4.1: Pseudohalogen chemistry with respect to comparison with halogens, preparation and uses- cyanogens, thiocyanogens and selenocyanogens.

# UNIT II: STEREOCHEMISTRY AND HYDROCARBON CHEMISTRY (15L)2.1: Stereochemistry 2.1.1: Isomerism: Types of isomerism; structural isomerism (chain, position and functional) and stereoisomerism. (1L)2.1.2: Chirality: Configuration, chirality and enantiomers, stereogenic / chiral centre, asymmetric carbon atom, representation of configuration by flying wedge formula and projection formulae - Fischer, Newmann and Sawhorse. (2L)2.1.3: Stereochemistry of carbon compounds with one and two similar and dissimilar asymmetric carbon atoms, enantiomers, diastereomers and racemic mixtures and their properties; threo, erythro and meso isomers. (2L)2.1.4: Geometrical isomerism due to restricted rotation around carbon – carbon double bond and cycloalkanes [disubstituted 3- and 4-membered cycloalkanes], E-Z nomenclature. (2L)2.1.5: Conformations; difference between conformation and configuration, conformations of ethane, propane and n-butane. (2L)2.2: Hydrocarbon Chemistry 2.2.1: Alkanes - mechanism of halogenation. (1L)2.2.2: Reactions of alkenes and cycloalkenes: hydrogenation, halogenation, addition of HX – Markovnikov and anti- Markovnikov additions with mechanism. (2L)2.2.3: Reactions of alkadienes – Diels-Alder reaction and 1,2- and 1,4- addition of X<sub>2</sub> [mechanism is not expected] (1L)2.2.4: Reactions of alkynes: hydration, addition of HX, selective hydrogenation to cisand trans- alkenes, acidity of terminal alkynes, preparation of metal acetylides and their alkylation. (2L)UNIT III: FUNCTIONAL GROUP CHEMISTRY (15 L)**3.1:** Reactions of alkyl halides with: aqueous alkali, alcoholic alkali (dehydrohalogenation), potassium cyanide, conversion of alkyl cyanide further to primary amine and carboxylic

acid, ammonia, silver salt of carboxylic acid, sodium alkoxide, Wurtz reaction.

(4L)

- 2<sup>nd</sup> Semester Syllabus for Core Component Course in Chemistry, St. Xavier's College –Autonomous, Mumbai.
- **3.2:** Reactions of alcohols with sodium metal, dehydration, esterification, oxidation of primary, secondary and tertiary alcohols. (2L)
- **3.3:** Reactions of aldehydes and ketones:
  - a) Addition to carbonyl compounds:
    - i) HCN and ii) NaHSO<sub>3</sub>
  - b) Condensation reaction with hydroxylamine
  - c) Oxidation with acidic K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> and PCC
  - d) Reduction of aldehydes and ketones:
    - i) catalytic reduction ii) Clemmensen reduction iii) reduction with LiAlH<sub>4</sub> and NaBH<sub>4</sub>
    - iv) Wolff Kishner reduction (4L)
- **3.4:** Reactions of carboxylic acids: Formation of salt [comparative 'acidity'], anhydride, amide, acid halide, ester and alkane. (2L)
- 3.5: Reactions of amines: Acetylation of amines with acetic anhydride and acetyl chloride, action of nitrous acid on primary / secondary / tertiary amines, alkylation of primary / secondary / tertiary amines yielding quaternary ammonium salts.(3L)
- **Note**: Each reaction should be studied with respect to compounds upto 6 carbon atoms. Based on these and the reactions of alkanes, alkenes and alkynes, multi-step synthesis of compounds having one functional group are expected, the number of carbon atoms in each being not more than six. No mechanisms are expected.

#### **REFERENCES:**

- 1. Organic Chemistry, R.T. Morrison and R.N. Boyd, 6<sup>th</sup> Edition, Pearson Education.
- 2. Organic Chemistry, T.W.G. Solomon and C.B. Fryhle, 8<sup>th</sup> Edition, John Wiley & Sons.
- 3. Organic Chemistry, Paula Y. Bruice, Pearson Education, 2008.
- 4. Organic Chemistry, John McMurray.
- 5. Organic Chemistry, L.G.Wade Jr.
- 6. Concise Inorganic Chemistry, J.D. Lee, 5<sup>th</sup> edition, Oxford Press.
- 7. Advanced Inorganic Chemistry, Volume I, S.Prakash, G.D. Tuli, S.K.Basu, R.D.Madan.
- 8. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, 3rd edition, 1977.
- 9. Inorganic Chemistry, James E. Huheey, 3rd edition, Harper & Row Publishers, Asia, Pte Ltd., 1983.
- 10. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford, 3rd edition, Oxford University Press,1999.
- 11. Theoretical Inorganic Chemistry, C. M. Day & J. Selbin, Affiliated East West Press Pvt. Ltd., 1985.
- 12. Advanced Inorganic Chemistry, Volume I and II, Bahl, Tuli and Anand.

CIA I: Objective and short answer questions 20 MARKS

CIA II : MCQ 20 MARKS

## **Template of Question Paper**

# FUNDAMENTALS OF INORGANIC AND ORGANIC CHEMISTRY II COURSE: S.CHE.2.02 OBJECTIVES

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL MARKS
1	10	06	04	20
II	10	06	04	20
III	04	08	08	20
TOTAL MARKS PER	24	20	16	60
OBJECTIVE				
% WEIGHTAGE	40	33	27	100

#### **END SEMESTER PAPER PATTERN:**

Total Marks: 60 Maximum Time: 2 hours

Total number of questions: 3 [all compulsory] of 20 marks each

1 question per unit.

Question set out of 26-28 marks with internal choice.

Sub questions of 2-3 marks.

#### PRACTICAL CHEMISTRY

Course No. S.CHE.2.PR

#### **LEARNING OBJECTIVES:**

- 1. To learn to perform experiments that have specific aims with the correct techniques.
- 2. To develop skills of observation, recording and analyzing data.
- 3. To learn to present the experimental work in a systematic manner.

**SEMESTER II: COURSE 3** 

Physico-Chemical Exercises Commercial Analysis

**SEMESTER II: COURSE 4** 

Organic Preparations Semi-micro Inorganic Qualitative Analysis

#### **COURSE 3:**

#### **VISCOMETRY:**

To determine co-efficient of viscosity of some organic liquids.

#### **STALAGMOMETRY:**

Determination of Surface Tension of some organic liquids.

#### **SEMI-MICRO INORGANIC QUALITATIVE ANALYSIS:**

Inorganic mixtures containing four radicals, 2 cations and 2 anions.

Preliminary dry tests, preparation of solution for analysis and wet tests for confirmation of the presence of the radicals.

#### **COURSE 4:**

#### **ORGANIC PREPARATIONS** [including calculation of yield and melting point]:

- i) Anhydride from Phthalic acid
- ii) Hydrolysis of amides
- iii) Bromination of acetanilide

#### **COMMERCIAL ANALYSIS:**

To determine the strength of commercial samples of antacid, vinegar, acetic acid and HCl [ standard succinic acid solution to be prepared by the students to standardize the given NaOH solution].

## **CIA AND END SEMESTER PRACTICAL EXAMINATION**

**COURSE 3:** Physico-Chemical Exercises + Commercial Analysis

**COURSE 4:** Organic Preparations +Semi-micro Inorganic Qualitative Analysis

**Journal:** 5 marks per course.

CIA: 15 marks per course.

**Duration:** 3 periods to be conducted during regular practicals by the faculty-in-charge. CIA for each course will be an exercise to test a practical skill (Qualitative and Quantitative).

**End Semester Examination:** 30 marks per course. This includes a 5 mark written test based on the theory behind all the experiments conducted per course.

**Duration:** 3 hours. Students are to perform two experiments (one per course).

**Batch Size:** Maximum 20 students per batch.



# St. Xavier's College – Autonomous Mumbai

# Syllabus for 3<sup>rd</sup> Semester Course in Chemistry (June 2015 onwards)

**Contents: Theory Syllabus for Courses:** 

S.CHE.3.01 - PHYSICAL AND ANALYTICAL CHEMISTRY I

S.CHE.3.02 - INORGANIC AND INDUSTRIAL CHEMISTRY I

S.CHE.3.03 - ORGANIC AND INDUSTRIAL CHEMISTRY I

PRACTICAL COURSE SYLLABUS FOR S.CHE.3.PR

# SYLLABUS UNDER AUTONOMY CHEMISTRY

# SEMESTER III COURSE: S.CHE.3.01 PHYSICAL AND ANALYTICAL CHEMISTRY I [45 LECTURES]

#### LEARNING OBJECTIVES

- 1. To understand some more concepts of thermodynamics from a chemist's viewpoint.
- 2. To predict the feasibility of a reaction.
- 3. To understand concepts involved in electrolytic cells and their applications.
- 4. To motivate students to solve numerical problems with different systems of units which illustrate the applicability of these concepts in chemistry.
- 5. To provide an introduction to analytical chemistry and information about latest developments in analytical techniques widely used in quality control and R&D of different types of chemical industries.

Unit I (15 L)

#### 1.1: Chemical Thermodynamics

- **1.1.1:** Recapitulation: Gibbs' free energy and Helmholtz free energy, Gibbs—Helmholtz equation (Derivation is not expected).
- **1.1.2:** Physical equilibrium involving pure substances, Clapeyron's equation and variation of vapour pressure with temperature, Clausius- Clapeyron equation and its application. partial molal properties with special reference to volume and free energy, introduction to chemical potential and its significance, Gibbs Duhem equation.
- **1.1.3:** Variation of chemical potential with pressure and temperature, fugacity, activity and their relationship with chemical potential, activity and activity coefficient.
- **1.1.4:** Techniques to achieve low temperature: (i) Joule-Thomson effect, concept of inversion temperature (Derivation is not expected), derivation of Joule -Thomson coefficient (ii) Adiabatic demagnetization technique.
- **1.1.5:** Thermodynamic derivation of Law of Mass Action,  $K_p$ ,  $K_c$  and their inter-relation, van't Hoff's reaction isotherm and reaction isochore.

#### 1.2: Self study

Numerical problems based on first and second law of thermodynamics, Gibbs' free energy and Helmholtz free energy, Gibbs - Helmholtz equation.

Unit II (15 L)

#### 2.1: Solutions of Electrolytes

**2.1.1:** Introduction of the terms involved: electronic and electrolytic conductors, conductivity, resistivity, specific resistivity, measurement of conductivity of solutions, conductometer, conductivity cell, cell constant, specific conductivity, molar conductivity and equivalent conductivity with their units in SI and C.G.S. systems.

**2.1.2:** Variation of molar conductivity with change in concentration of solution for strong and weak electrolytes. Arrhenius theory and Ostwald's dilution law for weak electrolytes.

Debye -Huckel theory for strong electrolytes (asymmetric and electrophoretic effect), concept of limiting molar conductivity.

- **2.1.3:** Kohlrausch's law of independent migration of ions.
- **2.1.4:** Applications of Kohlrausch's law: (i) Determination of limiting molar conductivity of weak electrolytes (ii) Determination of dissociation constant of a weak acid (iii) Determination of solubility of sparingly soluble salts.
- **2.1.5:** Migration of ions, transport number, determination of transport number by i) Hittorf's method using unattackable electrodes (only qualitative explanation) ii) Moving boundary method. Use of coulometer, factors affecting the transport number of ions, relation between transport number and ionic conductivity of an ion.
- 2.1.6: Relationship between ionic mobility and ionic conductivity of an ion (Derivation is not expected).

#### 2.2: Self study

Numerical problems based on all the above concepts.

## Unit III Basic concepts of Analytical Chemistry

(15 L)

#### 3.1: Introduction to Analytical Chemistry

(9L)

- **3.1.1:** Scope and importance of analytical chemistry, analytical chemistry and chemical analysis, classification of analytical methods, classical and instrumental techniques, destructive and non-destructive testing, qualitative and quantitative analysis an overview (introductory concepts only).
- **3.1.2:** Steps involved in chemical analysis: selection of a method for analysis, obtaining a sample: sampling, importance of sampling, terms involved in sampling, sampling techniques, purpose of sampling, types of sample and sampling, pre-treatment, measurement, calculation, evaluation and presentation of results.

#### 3.2: Use of Instrumental methods in Titrimetric analysis

(6L)

#### 3.2.1: Conductometric titrations

Basic principles, experimental set up, titration curves in the titration of:

(i) strong acid vs. strong base (ii) weak acid vs. strong base (iii) weak acid vs. weak base (iv) mixture of strong and weak acids vs. strong base (v) sodium chloride vs. silver nitrate (vi) barium hydroxide vs. magnesium sulphate. Advantages and limitations.

#### 3.2.2: Potentiometric titration

Principle, concept of indicator electrode and different types of graphical methods to determine the equivalence point.

#### 3.3: Self-study

Application of analytical methods in various fields such as chemical and pharmaceutical industries, environmental analysis and monitoring.

#### **REFERENCES:**

- 1. The Elements of Physical Chemistry: P.W. Atkins (1996) 2nd Ed., Oxford University Press, Oxford.
- 2. Physical Chemistry: G.M. Barrow 6th Ed, Tata McGraw Hill Publishing Co. Ltd., New Delhi.
- 3. Physical Chemistry: G.K. Vemulapalli (1997) Prentice Hall of India Pvt. Ltd., New Delhi.
- 4. Physical Chemistry: G.W. Castellan, 3rd Ed., Narosa Publishing House, New Delhi.
- 5. Text Book of Physical Chemistry, S. Glasstone, Affiliated East-West Press Pvt. Ltd., New Delhi.
- 6. Thermodynamics for Chemist: S. Glasstone, Affiliated East-West Press Pvt. Ltd., New Delhi.
- 7. Physical Chemistry: K.J. Laidler and J.H. Meiser, 2nd Ed.(First Indian Ed.1999) CBS Publishers and Distributors, New Delhi.
- 8. Physical Chemistry: Ira N. Levine (1995), 4th Ed., McGraw Hill, Inc.
- 9. Phase equilibria Reisman Arnold, Edited by Ernest M. Loebe, New York and London Academic Press.
- 10. Phase Rule: F.D. Ferguson and P.K. Jones (Butterworth Publisher).
- 11. Properties of Liquids and Solutions: J.N. Murrell and E.A. Boucher, Wiley, 1982.
- 12. Introduction to Principles of Heterogeneous Catalysis: Thomas J.M. and Thomas W.J.
- 13. An Introduction to Electrochemistry Samuel Glasstone, Affiliated East-West Press.
- 14. Modern Electrochemistry: J. O'M Bokris and A.K.N. Reddy, Maria Gamboa Aldeco, 2nd Ed, 1st Indian reprint, Springer (2006).
- 15. Principles and Applications of Electrochemistry: D.R.Crow, 4th Ed., Blackie, London, (1994).
- 16. Instrumental Methods of Chemical Analysis: Chatwal and Anand, 5th Ed., Himalaya Publication.
- 17. 2000 Solved Problems in Physical Chemistry: S.R.Metz, Tata McGrow Hill Publishers, New Delhi.
- 18. A Textbook of Physical Chemistry, K.L. Kapoor, MacMillan India Ltd.
- 19. Physical Chemistry: N.B.Singh, Shiva Saran Das, Rmji Singh, New Age International Pvt. Ltd., Publishers, New Delhi (2003).
- 20. D. A. Skoog, D.M.West, F.J.Holler, Fundamantal Analytical Chemistry, , 7th Ed. Philadelphia, Saunders College Publishing, 1996.
- 21. G.D.Christian, Analytical Chemistry, 6th Ed., John Wiley & Sons, New York, 2003.
- 22. J.G.Dick, Analytical Chemistry, International Student's Edition, McGraw Hill, Kogakusha Limited, New Delhi, 1973.

# **CIA I: Short answer questions**

20 MARKS

CIA II: Assignment+

20 MARKS

C1.	Xavier		C 11		TA /E	1 .
<b>ST</b>	x avier	. 6 1	n n	POP	- IVIII IN	กลา

Dept. of -----

#### ASSESSMENT OF WRITTEN ASSIGNMENT

NAME OF STUDENT: TITLE OF ASSIGNMENT:

**Assessment Grid**: Place one tick in each appropriate row. Overall mark should reflect the positions of ticks in the individual rows

100	ASSIGNMENT	80-100%	60-80%	40- 60%	20-40%	0-20%
		(17 -20Marks)	(13-16	(9-12	( 5-8 Marks)	(0-4 Marks)
			Marks)	Marks)		
30 %	ORGANISATION	Effective Presentation, Logical Format, Clear Statement of Ideas, Relevant Details, sequence of information and ideas could be easily followed	Few Problems	Many problems	Inadequate presentation, Ineffective format, Ineffective Communication of Ideas, Lack Relevant Details – But an attempt	No Attempt to or gamise
60%	CONTENT	Excellent - Impression of wide reading (research), good knowledge and comprehensive understanding Evidence of thoughtful input. Ability to critique, Bibliography mentioned.	Good	Satisfactory	Poor	V ery Poor
5%	VOCABULARY	Richness of V ocabulary	Very good range of vocabulary with some errors	Good range of vocabulary with some errors	Small range of vocabulary with errors	Little or no effort has been made to demonstrate vocabulary knowledge
5%	GRAMMAR, SPELLINGS, MECHANICS	Grammar, Spellings, Punctuations Correct.	Very Few Errors	Some Errors	Many Errors	No effort

COMMENTS:	_ OUT OF 20
NAME OF FACULTY MEMBER:	
SIGNATURE:St. Xavier's College, Mumbai	
Dept. of	

# **Template of Question Paper**

# PHYSICAL AND ANALYTICAL CHEMISTRY I COURSE: S.CHE.3.01 OBJECTIVES

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL
				MARKS
I	5 - 7	6 - 8	7 - 9	20
II	5 - 7	6 - 8	7 - 9	20
III	6 - 8	6 - 8	6 - 8	20
TOTAL	16 - 22	18 - 24	20 - 26	60
MARKS				
PER				
<b>OBJECTIVE</b>				
%	27 – 37	30 – 40	37 – 43	100
WEIGHTAGE				

## **END SEMESTER PAPER PATTERN:**

Total marks: 60 Maximum Time: 2 hours

Total number of questions: 3 [all compulsory] of 20 marks each

1 question per unit.

Questions set out of 30 marks [50 % internal choice]

Sub questions will not exceed 5 marks.

\*

SEMESTER III COURSE: S.CHE.3.02

#### INORGANIC AND INDUSTRIAL CHEMISTRY I

[45 LECTURES]

#### **LEARNING OBJECTIVES**

- 1. To introduce students to the basic concepts involved in chemical bonding.
- 2. To help students to determine the shape of a molecule by applying VSEPR theory.
- 3. To encourage students to analyze and integrate concepts relevant to inorganic chemistry required to understand compound formations with special reference to Valence Bond Theory and Molecular Orbital theory.
- 4. To enable students to understand the theories of Acids and Bases.
- 5. To expose students to principles of Gravimetric Analysis.

# **UNIT I: Chemical Bonding**

(15 L)

#### 1.1: Basics Of Chemical Bonding

- 1.1.1: Types of bonds: Ionic bond, covalent bond, single and multiple bonding, coordinate bond, sigma and pi-bonds, metallic bonds.
- 1.1.2: **Ionic bond:** Formation of ionic solids, lattice energy, solvation energy, Born-Haber cycle, Kapustinskii's equation (numerical problems expected).
- 1.1.3: Structures of some simple ionic solids like alkyl halides and stability of ionic structures based on radius ratio rules.
- 1.1.4: **Covalent bond:** Writing Lewis structures, formal charge and Lewis structures, concept of resonance and resonance energy, exceptions to the octet rule, bond enthalpy.
- 1.1.5: Sidgwick -Powell Theory.
- 1.1.6: **VSEPR concept:** Effect of lone pairs, effect of electronegativity, isoelectronic principle, shapes of chemical species on the basis of VSEPR theory.
- 1.1.7: **Metallic bond:** Theories of bonding in metals and free electron theory. MO or band theory, conductors, insulators and semiconductors.

# **UNIT II: Theories Of Chemical Bonding**

(15L)

## 2.1: Valence Bond Theory

(8L)

- 2.1.1: Hybridisation: sp<sup>3</sup>, sp<sup>2</sup>, sp hybridization of carbon and nitrogen, sp<sup>3</sup> and sp<sup>2</sup> hybridization of oxygen in organic compounds; theory of hybridization with respect to equivalence of contributing atomic orbitals in the following examples: CH<sub>4</sub>, NH<sub>3</sub> and H<sub>2</sub>O.
- 2.1.2: Energetics of hybridization, types of hybridization and extent of d-orbital participation in molecular bonding. sp,  $sp^2$ ,  $sp^3$ ,  $sp^3d^2$ ,  $sp^3d^3$  and sd with illustrations like BeCl<sub>2</sub>, BF<sub>3</sub>, SiCl<sub>4</sub>, PCl<sub>5</sub>, SF<sub>6</sub>, IF<sub>7</sub>, ClF<sub>3</sub>, ICl<sub>2</sub>, BrF<sub>5</sub>, SO<sub>2</sub>, SO<sub>3</sub> and BaCl<sub>2</sub>.
- 2.1.3: Merits and Demerits of Valence Bond Theory.

## 2.2: Molecular Orbital Theory [M.O.T.]

(7L)

- 2.2.1: Conditions for the formation of Molecular Orbitals.
- 2.2.2: Linear Combination of Atomic Orbitals to obtain Molecular Orbitals [LCAO-MO] Approach.
- 2.2.3: Application of the LCAO-MO to the formation of:
  - i) Homo- and Hetero-nuclear diatomic molecules and ions e.g. H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, F<sub>2</sub>, He<sub>2</sub>, Li<sub>2</sub>, Be<sub>2</sub>, C<sub>2</sub>, Ne<sub>2</sub>, CO, NO, HCl, HF and CN<sup>-</sup>.
  - ii) Occurrence of the Molecular ions  $O_2^+$ ,  $O_2^{1-}$ ,  $O_2^{2-}$ .

Discussion should include orbital interaction, stabilization of orbitals, bond order and with stability, bond length, bond energy and magnetic properties.

UNIT III (15 L)

#### 3.1: Theories of Acids and Bases

(10L)

- 3.1.1: Recapitulation of Arrhenius theory.
- 3.1. 2: Lowry-Bronsted concept: Bronsted acids and bases, acid-base properties of water, pH, strength of acids and bases, weak acids and acid ionization constants, weak bases and base ionization constants, relationship between ionization constants of acids and their conjugate bases, diprotic and polyprotic acids.
  - Solvent levelling, solvent-system definition of acids and bases.
  - Lux-Flood, Lewis & Usanovich concept.
- 3.1.3: Lewis acid concept: Examples of Lewis acids and bases, characteristics of Lewis acids. Pearsons concept of Hard and Soft Acids and Bases (HSAB), applications of HSAB.
- 3.1.4: Applications of acid-base chemistry: Superacids and superbases, heterogeneous acid-base reactions.

#### 3.2: Gravimetric Analysis

(5 L)

- 3.2.1: Definition and Types of Gravimetric Analysis.
- 3.2.2: Precipitation Gravimetry with respect to theory and practice.
  - (i) Solubility considerations: Common ion effect, diverse ion effect, pH and temperature.
  - (ii) Controlling particle size with respect to nucleation and rate of crystal growth.
- 3.2.3: Treatment of precipitates in Gravimetry: Digestion, Filtration and Washing, Drying and Ignition.
- 3.2.4: Use of Organic Reagents in Gravimetric analysis e.g. Dimethyglyoxime, Salicylaldoxime, Cupron, Oxine and Cupferron.

#### **REFERENCES:**

- 1. Chemistry, Raymond Chang, 9<sup>th</sup> edition, Tata McGraw Hill.
- 2. Chemistry Concepts and Connections, Charles H. Corwin, Prentice Hall.
- 3. Chemistry, James E. Brady, Neil D. Jespersen and Alison Hyslop, 6<sup>th</sup> edition.
- 4. Chemistry, McMurry Fay, Prentice Hall.
- 5. Shriver Atkins Inorganic Chemistry, P. W. Atkins, Overton, Rourke Weller, Armstrong, 5<sup>th</sup> edition, Oxford University Press.
- 6. Advanced Inorganic Chemistry, Bahl, Anand & Tuli, Vol 1 & 2.

- 7. Vogel's tesxtbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6<sup>th</sup> edition.
- 8. Fundamental Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler, 8th edition.
- 9. Inorganic Chemistry, P. A. Cox, Bios Scientific Publishers Ltd.
- 10. Basic Concepts of Analytical Chemistry, S. M. Khopkar, 3<sup>rd</sup> edition, New Age International Publication.
- 11. Concise Inorganic Chemistry, J.D. Lee, 5th edition, Oxford University Press.
- 12. Inorganic Chemistry, James E. Huheey, 3<sup>rd</sup> edition, Harper & Row Publishers, Asia, Pvt. Ltd., 1983.

CIA I: Short answer questions / MCQ

20 MARKS

**CIA II: Problem solving / Presentations** 

20 MARKS

#### **Template of Question Paper**

#### INORGANIC AND INDUSTRIAL CHEMISTRY I

#### **COURSE: S.CHE.3.02**

#### **OBJECTIVES**

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL
				MARKS
I	6-8	6-8	6-8	20
II	6-8	6-8	6-8	20
Ш	6-8	6-8	6-8	20
TOTAL	18-24	18-24	18-24	60
MARKS PER				
<b>OBJECTIVE</b>				
%	30 – 40	30 – 40	30 – 40	100
WEIGHTAGE				

#### **END SEMESTER PAPER PATTERN:**

Total Marks: 60 Maximum Time: 2 hours

Total number of questions: 3 [all compulsory] of 20 marks each.

1 question per unit.

Questions set out of 30 marks [50% internal choice].

Sub questions will not exceed 5 marks.

\*

SEMESTER III COURSE: S.CHE.3.03

#### ORGANIC AND INDUSTRIAL CHEMISTRY I

[45 LECTURES]

## **Learning Objectives:**

- 1. To understand the mechanism of reactions involving the reactive intermediates.
- 2. To introduce the concepts of aromatic, non aromatic and anti aromatic compounds.
- 3. To study the mechanism of aromatic electrophilic substitution and the effect of substituents on the orientation of an incoming electrophile.
- 4. To familiarize the students with preparation, reactions and applications of aromatic hydrocarbons, haloarenes, phenols, ethers and epoxides and understand mechanisms of certain reactions.
- 5. To introduce the aspects of a chemical plant and study the sources and classification of fuels.

UNIT I (15 L)

#### 1.1: Mechanism of Organic reactions

(6L)

The mechanism of reactions involving the following reactive intermediates:

**1.1.1:** Carbocations: Different types of carbocations such as alkyl, allyl, benzyl.

 $S_{N}\mathbf{1}$  reaction. Electrophilic addition across an olefinic double bond.

Rearrangements: Wagner-Meerwein rearrangement, Pinacole-Pinacolone rearrangement.

- **1.1.2:** Carbanions: Concept of carbon acid. Alkylation of carbon acids (active methylene compounds and terminal alkynes) using alkyl halides and synthetic applications of these reactions. Reactions of Grignard reagents at sp<sup>3</sup>carbon and carbonyl group. Aldol condensation with mechanism.
- **1.1.3:** Carbon radicals: General reactions of radicals abstraction, addition to C=C, combination, disproportionation. Addition of HBr to alkenes in presence of peroxide. Polymerization.
- **1.1.4:** Carbenes: Generation of carbenes through alpha elimination, from diazoalkanes, from ketenes. Structure and stability of carbenes. Reactions: insertion into C-H bond and addition to olefin.

# 1.2: Tautomerism: (1L)

Keto-enol tautomerism in aldehydes and ketones, acid and base catalysed enolisation, enol content and stabilized enols:  $\beta$  –ketoesters,  $\beta$ -diketones, phenols.

# 1.3: Aromatic Electrophilic Substitution Reaction:

- **1.3.1:** Electronic structure and Huckel's Rule of aromaticity and its applications to carbocyclic and heterocyclic compounds, benzenoid and non-benzenoid compounds and ions including nomenclature of aromatic systems.
  - Concept of anti-aromaticity, non- aromaticity.
- **1.3.2:** General mechanism of aromatic electrophilic substitution reaction with energy profile diagram.
- **1.3.3:** Drawing resonance structures of mono-substituted benzenes activated and deactivated aromatic rings.

(8L)

**1.3.4:** Effect of electron-withdrawing and electron-donating substituents on the orientation of an incoming electrophile on the basis of – (i) electron-density distribution (ii) stability of intermediate. Cases to be studied: Mono and disubstituted benzenes containing - alkyl, amino, hydroxyl, alkoxy, halo, acyl, nitro, carboxy groups, ortho / para ratio.

UNIT II (15 L)

#### 2.1: Aromatic Hydrocarbons

(3L)

- **2.1.1:** Structures of benzene, naphthalene, linear and angular arenes.
- **2.1.2:** Alkyl arenes: Preparation of alkyl arenes through reforming, Friedel-Crafts alkylation (with mechanism), using olefins, alcohols, alkyl halides.
- **2.1.3:** Reactions of alkyl arenes side-chain oxidation, ring vs side-chain halogenation (mechanism).

2.2: Haloarenes (4L)

- **2.2.1:** Preparations of haloarenes. Halogenation of arenes Halogenation of benzene and substituted benzenes with molecular halogens (mechanism), limitations.
- **2.2.2:** Reactions of haloarenes: Lack of reactivity of aryl halides under  $S_N1$  and  $S_N2$  reaction conditions. General mechanism (addition-elimination) of aromatic nucleophilic substitution reaction with energy profile diagram. Effect of substituents on the reaction hydrolysis and amination of haloarenes. Benzyne intermediate mechanism (elimination-addition) of aromatic nucleophilic substitution reaction . Grignard reagent formation. Ullmann reaction.
- **2.2.3:** Applications of aromatic halogen compounds.

2.3: Phenols (3L)

- **2.3.1:** Preparation of phenols: Preparation from (i) halobenzenes (ii) from aromatic sulfonic acids (benzene and naphthalene sulfonic acids) (iii) isopropyl and 2-butylbenzene by hydroperoxide method.
- **2.3.2:** Reactions of phenols: Acidity of phenols effect of substituents on acidity of phenols. Salt Formation. Etherification direct reaction with alcohol. Williamson synthesis. O-acylation. Halogenation, Nitration, Fries rearrangement of aryl carboxylates, Claisen rearrangement of allyloxyarenes.
- **2.3.3:** Applications of phenols.

2.4: Ethers (3L)

- **2.4.1:** Preparation: Dehydration of alcohols (mechanism), reactions of phenols with alcohols, Williamson synthesis (mechanism).
- **2.4.2:** Reactions: Acid-catalyzed cleavage reaction with HX (mechanism).
- **2.4.3:** Applications: Applications of ethers, Crown ethers: Structure of 12-crown-4 and 18-crown-6 and their uses.

2.5: **Epoxides:** (2L)

**2.5.1:** Preparation: Oxidation of olefins – ethylene oxide. Reaction of peracids with olefins; from vicinal halohydrins.

- **2.5.2:** Reactions: Reactivity. Ring opening reactions by nucleophiles
  - (a) in acidic conditions, hydrolysis, reaction with HX, alcohol, HCN.
  - (b) In neutral or basic conditions: ammonia, amines, metal cyanides, Grignard reagents, alkoxides.
- **2.5.3:** Applications of epoxides (including chiral epoxides).

UNIT III (15 L)

#### 3.1: Chemical Industry

(4L)

**3.1.1:** Introduction to aspects of a chemical plant, terminology [raw materials, intermediates, end products, by-products, waste-products], unit operations, unit processes [single and multiple], batch and continuous operations, block diagrams, flow diagrams.

#### 3.2: Sources of Organic Compounds

(7L)

- **3.2.1:** Introduction
- **3.2.2:** Solid eg. Destructive Distillation, Coal Tar Refining.
- **3.2.3:** Liquid eg. Petroleum: characteristics, refining of petroleum [applying block / flow diagrams to unit processes involved in refining like cracking].
- **3.2.4:** Gaseous eg. Natural gas: production, conversion to methanol [manufacturing process].
- **3.2.5:** Renewable Sources (i) conversion of biomass into chemicals (ii) biofuels: types and brief description of a few representative examples [bioethanol, biodiesel].

#### 3.3: Manufacture of Bulk Chemicals

(4L)

**3.3.1:** Phenol, styrene and dodecylbenzene [including reactions and reaction conditions, block / flow diagram, description].

#### **REFERENCES:**

- 1. Organic Chemistry, Francis A Carey, Pearson Education, 6th Edition, Special Indian Education, 2008.
- 2. Organic Chemistry, R.T. Morrison and R.N. Boyd, 6th Edition, Pearson Education.
- 3. Organic Chemistry, T.W.G. Solomon and C.B. Fryhle, 8th Edition, John Wiley & Sons, 2004.
- 4. Fundamentals of Organic Chemistry, G. Marc Loudon, 4th Edition, Oxford University Press, 2006.
- 5. Organic Chemistry, L.G. Wade Jr. and M.S. Singh, 6th Edition, Pearson Education, New Delhi, 2008.
- 6. Organic Chemistry, Paula Y. Bruice, Pearson Education, 2008.
- 7. Organic Chemistry, J.G. Smith, 2nd Edition, Special Indian Edition, Tata McGraw Hill, New Delhi, 2008.
- 8. Organic Chemistry, S.H. Pine, McGraw Hill Kogakusha Ltd.
- 9. Organic Chemistry, J. McMurry, 5th Edition, Asian Books Pvt. Ltd., New Delhi, 2000.
- 10. Organic Chemistry, S. Ege, A.I. T.B.S., 3rd Edition, Publishers, New Delhi, 1999.
- 11. A guide to mechanism in Organic Chemistry, 6th Edition, Peter Sykes, Pearson Education, New Delhi.
- 12. Organic Reaction Mechanism, 3<sup>rd</sup> Ed., V.K. Ahluwalia and R.K. Parashar, Narosa Publications.

- 13. Stereochemistry, P.S. Kalsi, New Age International Ltd., 4th Edition, 2006.
- 14. Stereochemistry of Carbon compounds, E. L. Eliel, Tata McGrawHill, New Delhi.
- 15. Environmental Chemistry, A.K.Ahluwalia, Ane Books India.
- 16. Organic Synthesis Special Techniques, V.K.Ahluwalia, Renu Aggarwal, Narosa Publication.
- 17. B. Pani, Textbook of Environmental Chemistry, I. K. International Publishing House Pvt. Ltd., New Delhi, (2007).
- 18. M. L. Srivastava, Environmental Chemistry, Shree Publishers & Distributors, New Delhi, (2004).
- 19. P. S. Sindhu, Environmental Chemistry, New Age International (P) Ltd., New Delhi, (2002).
- 20. An introduction to Green Chemistry, V.K. Ahluwalia, Vishal Publishing Co.
- 21. University Chemistry, Bruce Mahan.
- 22. Fundamental concepts of Environmental Chemistry, G.S.Sodhi
- 23. Biomass for Renewable Energy, Fuels & Chemicals: Donald L. Klass, Academic Press, London, UK.

**CIA I:** Short answer questions

20 MARKS

**CIA II: Short answer questions** 

20 MARKS

# **Template of Question Paper**

ORGANIC AND INDUSTRIAL CHEMISTRY I

COURSE: S.CHE.3.03

#### **OBJECTIVES**

UNIT	KNOWLEDG	UNDERSTANDING	APPLICATION	TOTAL
	${f E}$			MARKS
I	7	7	6	20
II	7	7	6	20
III	7	7	6	20
TOTAL MARKS	21	21	18	60
PER OBJECTIVE				
% WEIGHTAGE	35	35	30	100

#### END SEMESTER PAPER PATTERN:

Total marks: 60 Maximum Time: 2 hours

Total number of questions: 3 [all compulsory] of 20 marks each.

1 question per unit.

Questions set out of 30 marks [50 % internal choice].

Sub questions will not exceed 5 marks.

#### PRACTICAL CHEMISTRY

Course No. S.CHE.3.PR

#### LEARNING OBJECTIVES

- 1. To learn to perform experiments that have specific aims with correct techniques.
- 2. To develop skills of observation, recording and analyzing data.
- 3. To learn to present the experimental work in a systematic manner.

#### **SEMESTER III:**

COURSE 1: PHYSICAL CHEMISTRY COURSE 2: INORGANIC CHEMISTRY COURSE 3: ORGANIC CHEMISTRY

#### **COURSE 1: PHYSICAL CHEMISTRY**

#### **CHEMICAL KINETICS:**

To study the reaction between KI and  $K_2S_2O_8$  using equal concentrations and unequal concentrations.

#### pH METRY:

pH metric titration of weak acid vs strong base and to determine pK<sub>a</sub> value.

#### **CONDUCTOMETRY:**

Conductometric titration of strong acid vs strong base.

Conductometric titration of weak acid vs. strong base.

#### **COURSE 2: INORGANIC CHEMISTRY**

#### **SEMI-MICRO QUALITATIVE ANALYSIS:**

Analysis of mixtures containing 2 cations and 2 anions. Dry tests and wet tests to be performed.

Anions: Cl<sup>-</sup>, Br<sup>-</sup>, NO<sub>2</sub><sup>-</sup>, NO<sub>3</sub><sup>-</sup>, CO<sub>3</sub><sup>2-</sup>, SO<sub>4</sub><sup>2-</sup>, PO<sub>4</sub><sup>3-</sup>, Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup>

At least 6 mixtures to be analyzed with interfering radicals. More emphasis to be placed on separation and detection of cations.

# **INORGANIC PREPARATIONS**

- 1. Synthesis of CuCl<sub>2</sub>. 2DMSO.
- 2. Preparation of (double salt) copper (II) ammonium sulfate (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>.CuSO<sub>4</sub>.6H<sub>2</sub>O.
- 3. Synthesis of (complex) Tetrammine Copper (II) Sulphate hydrate [Cu(NH<sub>3</sub>)<sub>4</sub>]SO<sub>4</sub>.H<sub>2</sub>O.
- 4. Preparation of Double salt (Mohr's salt).

## **COURSE 3: ORGANIC CHEMISTRY**

- **1. Derivative preparation:** The exercise is aimed at imbibing the concept of derivative preparation as a method of identifying a given compound from a set of compounds having the same functional group. Based on the m.p. identify the given compounds looking at the chart. About 500 mg of a suitable compound be given. The candidate will prepare the given derivative. Crystallization is expected. M.P. of the dried derivative should be taken and appropriate inference drawn. The derivative preparation should involve one of the following reactions: (a) oxime preparation (b) nitration of aromatic compounds (c) N/O-acylation (d) Schiff base preparation (e) 2,4-DNP hydrazone formation (f) oxidation of aromatic compounds.
- **2. Estimation of an Organic Compound:** The following estimations be given:
- a) Estimation of formaldehyde by oxidation using iodine and alkali.
- b) Estimation of aniline by bromination using brominating solution.
- c) Estimation of acetamide by hydrolysis.
- d) Saponification Value of the given oil.

### Note:

- (1) A minimum of three estimations be done by the candidates.
- (2) For the estimations, the concentrations and the quantities be reduced. For dilution a standard flask of 100 cm<sup>3</sup> capacity and for the transfer a pipette of 10 cm<sup>3</sup> capacity be used. The concentrations of the solutions be around 0.05N.

## **\*** CIA AND END SEMESTER PRACTICAL EXAMINATION

Course 1: Physical Chemistry - Exercise to test practical skills.

Course 2: Inorganic Chemistry - Exercise to test practical skills, qualitative /quantitative.

**Course 3: Organic Chemistry** - Exercise to test practical skills, qualitative /quantitative.

Journal: 5 marks per course.

CIA: 15 marks per course.

**Duration**: 4½ periods to be conducted during regular practicals by the faculty-in- charge.

One or more practical skill will be tested in the CIA.

**End Semester Examination**: 30 marks per course. This includes a 5 mark written test based on the theory behind all the experiments conducted per course.

**Duration**: 3 hrs per course. To be conducted at the end of the semester.

Batch size: Maximum 20 students per batch.

\*



## St. Xavier's College – Autonomous Mumbai

# Syllabus for 4<sup>th</sup> Semester Course in Chemistry (June 2015 onwards)

**Contents: Theory Syllabus for Courses:** 

S.CHE.4.01 - PHYSICAL AND ANALYTICAL CHEMISTRY II

S.CHE.4.02 - INORGANIC AND INDUSTRIAL CHEMISTRY II

S.CHE.4.03 - ORGANIC AND INDUSTRIAL CHEMISTRY II

PRACTICAL COURSE SYLLABUS FOR S.CHE 4 PR

## SYLLABUS UNDER AUTONOMY CHEMISTRY

SEMESTER IV COURSE: S.CHE.4.01

## PHYSICAL AND ANALYTICAL CHEMISTRY II

[45 LECTURES]

## **LEARNING OBJECTIVES**

- 1. Introducing the concept of phase rule to understand the behaviour of heterogeneous systems.
- 2. To understand basic principles involved in separation of liquid mixtures by distillation.
- 3. To understand the concept of steam distillation and its applications.
- 4. To give latest information and understanding of different types of electrodes used in various galvanic cells.
- 5. To understand Beer Lambert's law and its applications in various quantitative as well as qualitative analysis and the experimental procedure of spectroscopy.
- 6. To motivate the students to solve numerical problems.
- 7. To encourage students to use computer software like spreadsheet to plot the appropriate graph and obtain accurate results from experimental data.

## **Unit I: Electrochemistry**

(15 L)

- **1.1:** Introduction to Electrolytic cell and Electrochemical cells (Galvanic /Voltaic cell).
- **1.2.1:** Ion selective and ion specific electrodes, comparison, simple examples. Types of ion specific electrodes: (i) Metal-metal ion electrode (ii) Gas electrode (including S.H.E.) (iii) Metal- metal insoluble salt electrode (including reference calomel electrode.) (iv) Redox electrode (v) Amalgam electrode.
- **1.2.2:** Cell representation of galvanic cell from cell reactions and vice versa. Concept of combination electrode: Glass electrode- construction and working (in brief).
- 1.3.1: Derivation of Nernst equation for the emf of a cell and hence for a single electrode potential, potential of glass electrode and quinhydrone electrode in terms of pH. Determination of equilibrium constant from EMF measurements. Thermodynamic parameters [ΔG, ΔH and ΔS] for the reaction taking place in a chemical cell.
- **1.3.2:** Introduction to electrode concentration cell and electrolyte concentration cell.
- 1.4: Introduction to pH metric titrations. Titration curves for:(i) strong acid vs. strong base (ii) weak acid vs. strong base. Determination of equivalence point from titration curves (pH vs V,  $\Delta$ pH/  $\Delta$ V vs. mean volume). Determination of K<sub>a</sub> for weak monobasic acid. Advantages and limitations of pH-metry.

**Self study:** Numerical problems on calculation of pH of different types of acids, bases and buffer solutions.

## **Unit II: Phases in Equilibria**

(15 L)

**2.1:** Introduction to the terms in Phase Equilibria Phase, components, degrees of freedom, Gibb's phase rule, phase diagram (with one suitable example).

## 2.2: Two component systems

- **2.2.1:** Completely miscible liquid-liquid mixtures: Phase diagrams of ideal mixture: vapour pressure composition and temperature composition diagrams. Raoult's law, ideal solutions. Deviation from Raoult's law, positive and negative deviations (Numerical Problems expected).
- **2.2.2:** Phase diagrams of non-ideal mixtures, azeotropes, distillation of azeotropic mixtures.
- **2.2.3:** Partially miscible liquid-liquid mixtures: only introduction and examples.
- **2.2.4:** Completely immiscible liquid-liquid mixtures: Steam distillation and its applications (Numerical Problems expected).

## 2.3: Physico-chemical aspect solvent extraction

Nernst distribution law: partition coefficient and distribution ratio, solute undergoing association and dissociation. Derivation of expression for amount of solute remaining unrestricted in the aqueous phase after multiple extractions with an organic solvent (Numerical Problems expected).

**Self study:** Additional numerical problems on above topics, one component system: CO<sub>2</sub> system, breaking of azeotropes.

## **Unit III: Visible Spectroscopy and Separation Techniques**

(15 L)

## 3.1: Visible spectroscopy

(6L)

- **3.1.1:** Recap: Terms involved: radiant power, absorbance, transmittance, wavelength of maximum absorption. Beer Lambert's Law [derivation expected], molar absorptivity Deviations from Beer –Lambert's law.
- **3.1.2:** Components of an optical instrument, photometer and spectrophotometer, construction and working of a single beam colorimeter.

## 3.1.3: Photometric titrations

Basic principles and titration curves. Advantages and Limitations.

## 3.2: Introduction to Separation Techniques

(7L)

## **3.2.1:** Solvent extraction

Principle, separation factor, criteria for selection of solvent.

## 3.2.2: Chromatography

Introduction to chromatographic techniques, basic principles, classification of chromatographic techniques.

## 3.3: Introduction to analytical method validation

(2L)

Performance characteristics of an analytical method: accuracy, precision, detection limit, dynamic range, sensitivity, selectivity, use of calibration curve for quantitative analysis.

**Self Study**: Applications of Colorimetry and numerical problems based on Spectroscopy.

### REFERENCES

- 1. The Elements of Physical Chemistry: P.W. Atkins (1996) 2nd Ed, Oxford University Press, Oxford.
- 2. Physical Chemistry: G.M. Barrow 6th Ed, Tata McGraw Hill Publishing Co. Ltd., New Delhi.
- 3. Physical Chemistry: G.K. Vemulapalli (1997)Prentice Hall of India Pvt. Ltd., New Delhi
- 4. Physical Chemistry: G.W. Castellan, 3rd ed., Narosa Publishing House, New Delhi.
- 5. Text Book of Physical Chemistry, S. Glasstone, Affiliated East-West press Pvt.Ltd., New Delhi.
- 6. Thermodynamics for Chemist: S. Glasstone Affiliated East-West Press Pvt. Ltd., New Delhi.
- 7. Physical Chemistry: K.J. Laidler and J.H. Meiser, 2nd ed.(First Indian ed.1999) CBS Publishers and Distributors, New Delhi.
- 8. Physical Chemistry: Ira N.Levine (1995), 4th ed., McGraw Hill, Inc
- 9. Phase equilibria Reisman Arnold, Edited by Ernest M. Loebe, New York and London Academic Press.
- 10. Phase Rule: F.D. Ferguson and P.K. Jones, (Bitterworth Publisher).
- 11. Properties of Liquids and Solution: J.N. Murrell and E.A. Boucher, Wiley, 1982.
- 12. Introduction to Principles of Heterogeneous Catalysis: Thomas J.M., and Thomas W.J. Academic, 1967.
- 13. An Introduction to Electrochemistry Samuel Glasstone Affiliated East-West Press.
- 14. Modern Electrochemistry: J. O'M Bokris and A.K.N. Reddy, Maria Gamboa Aldeco, 2nd ed, 1st Indian reprint, Springer, (2006).
- 15. Principles and Applications of Electrochemistry: D.R.Crow, 4th ed., Blackie, London, (1994).
- 16. Instrumental Methods of Chemical Analysis: Chatwal and Anand, 5th ed., Himalaya Publication.
- 17. 2000 Solved Problems in Physical Chemistry : S.R.Metz, Tata McGraw Hill Publishers, New Delhi.
- 18. A Textbook of Physical Chemistry, K.L. Kapoor, MacMillan India Ltd.
- 19. Physical Chemistry: N.B.Singh, Shiva Saran Das, Rmji Singh, New Age International Pvt. Ltd., Publishers, New Delhi. (2003).
- 20. D. A. Skoog, D.M.West, F.J.Holler Fundamantal Analytical Chemistry, , 7th ed. Philadelphia, Saunders college Publishing, 1996
- 21. G.D.Christian, Analytical Chemistry, 6th ed. John Wiley &Sons, new York, 2003.
- 22. J.G.Dick, Analytical Chemistry, International Student's Edition, McGraw Hill, Kogakusha Limited, New Delhi, 1973.

CIA I: Short answer questions 20 MARKS

CIA II: Numerical Problems 20 MARKS

## **Template of Question Paper**

## PHYSICAL AND ANALYTICAL CHEMISTRY II COURSE: S.CHE.4.01

## **OBJECTIVES**

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL
				MARKS
I	5 - 7	6 - 8	7 - 9	20
II	5 - 7	6 - 8	7 - 9	20
III	6 - 8	6 - 8	6 - 8	20
TOTAL MARKS	16 - 22	18 - 24	20 - 26	60
PER		_		
OBJECTIVE				
%	27 – 37	30 - 40	37 – 43	100
WEIGHTAGE				

## **END SEMESTER PAPER PATTERN:**

Total Marks: 60 Maximum Time: 2 hours

Total number of questions: 3 [all compulsory] of 20 marks each

1 question per unit

Questions set out of 30 marks [50 % internal choice]

Sub questions will not exceed 5 marks

## SYLLABUS UNDER AUTONOMY CHEMISTRY

SEMESTER IV COURSE: S.CHE.4.02

## INORGANIC AND INDUSTRIAL CHEMISTRY II

[45 LECTURES]

## **LEARNING OBJECTIVES**

- 1. To introduce students to Co-ordination Chemistry, elucidating concepts like the theories involved in "bonding" and features of coordination compounds.
- 2. To introduce students to organometallic compounds.
- 3. To understand a few bioinorganic molecules.
- 4. To introduce students to the basic concepts involved in metallurgy and corrosion.
- 5. To study Environmental Chemistry with reference to some common pollutants.

UNIT I: (15L)

## 1.1: Co-ordination Chemistry

(8L)

- 1.1.1: Introduction to Co-ordination Compounds. Distinction between Double salts and Co-ordination compounds.
- 1.1.2: Terms involved in Co-ordination Chemistry: Co-ordination Compound, central metal atom or ions, complex compound, Complex ion, Ligand: Definition, Classification, Chelates and chelating agents, Co-ordination Sphere, Co-ordination Number, Charge of the complex ion, calculation of oxidation and coordination number of metal etc.
- 1.1.3: Werner's Theory postulates.
- 1.1.4: IUPAC nomenclature of Co-ordination compounds.
- 1.1.5: Sidwick Model (Eighteen electron rule), EAN rule limitations.
- 1.1.6: Isomerism in Co-ordination compounds:

  Structural isomerism (ionization, hydrated, linkage ligand, coordination position, polymerization isomers) and Geometrical isomerism and optical isomerism.

## **1.2:** Bonding in Co-ordination Compounds:

(7L)

- 1.2.1: Pauling's Valence Bond Theory Assumptions, concept of hybridization, Limitations and Drawbacks.
- 1.2.2: Bonding in tetrahedral, square planer, trigonal bipyramidal and octahedral complexes with examples.
- 1.2.3: Inner and outer orbital complexes.
- 1.2.4: Electroneutrality principle and Back (Multiple) bonding.
- 1.2.5: Applications of Co-ordination Compounds (complexes) in different fields

UNIT II: (15L)

## 2.1: Organometallic Compounds

(7L)

- 2.1.1: Introduction to Organometallic compounds and Definition.
- 2.1.2: Classification on the basis of Hapticity and Nature of Metal Carbon bond.
- 2.1.3: 18-electron rule and its application to: carbonyls (including carbonyl hydrides and carbonylates), nitrosyls, cyanides, metal-carbon sigma and pi-bonded organometallics of transition metals.
- 2.1.4: Classification of metal carbonyls: Mononuclear, polynuclear, non-bridged and bridged carbonyls. General methods of preparation of carbonyls. Molecular orbital configuration of CO molecule. CO molecule acts as terminal and bridging carbonyl group.

## 2.2: Bioinorganic Chemistry:

(8L)

- 2.2.1: Essential and trace elements in biological processes; Role of metal in bioinorganic chemistry (Na+,K<sup>+</sup>,Ca<sup>2+</sup>,Mg<sup>2+</sup>,Fe<sup>3+</sup>/Fe<sup>2+</sup>,Cu<sup>2+</sup>/Cu<sup>+</sup>,Zn<sup>2+</sup>).
- 2.2.2: Metalloporphyrins with special reference to active site structures and biofunctions of cytochromes and Heme proteins-myoglobin and haemoglobin. Functions of oxygen transfer, Fe (II) complex of porphyrin, oxygen binding O<sub>2</sub> transfer, partial pressure, pH dependence. Nature of oxyheamoglobin and deoxyheamoglobin, geometry of complex.
- 2.2.3: Photosynthesis PS-I and PS-II.
- 2.2.4: Metal ion induced toxicity and chelation therapy; metal ions as drugs (cisplatin and a few gold drugs).

## **UNIT III: Industrial Inorganic Chemistry:**

(15L)

- 3.1: Corrosion (5L)
- 3.1.1: Introduction to Corrosion [including the economics and importance of corrosion].
- 3.1.2: Types of Corrosion.
- 3.1.3: Electrochemical Theory of Corrosion.
- 3.1.4: Methods of Protection of Metals : (i) Coating (ii) Electroplating (iii) Cathode Protection (iv) Anodizing (v) Sacrificial Coating.
- 3.1.5: Passivity of metals: Definition, Theories of passivity (i) oxide film theory (ii) Gaseous film theory (iii) Physical film theory, valence theory, catalytic theory, Allotropic theory, electrochemical passivity.

## 3.2: Environmental Chemistry

(5 L)

- 3.2.1: Basic properties of chemicals in the environment.
- 3.2.2: Environmental transformations and degradation processes.
- 3.2.3: Contaminants in the environment- pesticides, soaps and detergents, organometallic compounds, polychlorinated biphenyls and dioxin.
- 3.2.4: Radioactive pollution.

3.3: Metallurgy (5L)

- 3.3.1: Metallurgical operations-Pulverisation, calcination, roasting and refining.
- 3.3.2: Physicochemical principles involved in hydrometallurgy, pyrometallurgy and electrometallurgy.

## **REFERENCES:**

- 1. Chemistry, Raymond Chang, 9<sup>th</sup> edition, Tata McGraw Hill.
- 2. Concise Inorganic Chemistry, J.D. Lee, 5<sup>th</sup> edition, Oxford University Press.
- 3. James E. Huheey, Inorganic Chemistry, 3<sup>rd</sup> edition, Harper & Row Publishers, Asia, Pvt Ltd., 1983.
- 4. Shriver Atkins Inorganic Chemistry, P. W. Atkins, Overton, Rourke Weller, Armstrong, 5<sup>th</sup> edition, Oxford University Press.
- 5. Introduction to coordination , solid state and descriptive inorganic chemistry, Glen E. Rogers.
- 6. Chemistry Science of change, 3<sup>rd</sup> edition, D.W. Oxtoby, W.A. Freeman, T.F. Block.
- 7. The Organometallic chemistry of transition metals, R.H. Crabtree, 5<sup>th</sup> edition, Wiley.
- 8. Fundamental transition metal, Organometallic chemistry, C.M. Lukehart.
- 9. Chemistry-The molecular science, J.W. Moore, C.L. Stanitski and P.C. Jurs, 3<sup>rd</sup> edition, Thomson Publishers.
- 10. Advanced Inorganic Chemistry, Bahl, Anand & Tuli, Vol 1 & 2.
- 11. Chemistry, McMurray and Fay.
- 12. Organometallic chemistry, R.C. Mehrotra and A. Singh.
- 13. Inorganic chemistry, Gary Wulfsberg.
- 14. Principles of Organometallic chemistry, 2<sup>nd</sup> edition, P. Powell.
- 15. Bionorganic Chemistry: Inorganic elements in the chemistry life, Wiley, 2<sup>nd</sup> edition, W. Kaim, B.Schwederski, A. Klein.
- 16. Environmental chemistry, Lewis publishers, D. W. Connell.
- 17. Inorganic Chemistry (Biological and environmental aspects), A.K. Das.
- 18. Metal ions in Biochemistry, Narosa Publishing House, P. K. Bhattacharya.
- 19. An introduction to electrochemistry, Samuel Glasstone.
- 20. Metallic corrosion passivity and protection, U. R. Evans.
- 21. Basics of corrosion chemistry, Norio Sato.
- 22. Extractive Metallurgy, Newton.

CIA I: Short answer questions 20 MARKS

CIA II: MCQ 20 MARKS

## **Template of Question Paper**

## INORGANIC AND INDUSTRIAL CHEMISTRY II COURSE: S.CHE.4.02

## **OBJECTIVES**

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL
				MARKS
I	6-8	6-8	6-8	20
II	6-8	6-8	6-8	20
III	6-8	6-8	6-8	20
TOTAL	18-24	18-24	18-24	60
MARKS PER				
OBJECTIVE				
%	30 – 40	30 – 40	30 – 40	100
WEIGHTAGE				

## **END SEMESTER PAPER PATTERN:**

Total Marks: 60 Maximum Time: 2 hours

Total number of questions: 3 [all compulsory] of 20 marks each.

1 question per unit.

Questions set out of 30 marks [50% internal choice].

Sub questions will not exceed 5 marks.

## SYLLABUS UNDER AUTONOMY CHEMISTRY

SEMESTER IV COURSE: S.CHE.4.03

## ORGANIC AND INDUSTRIAL CHEMISTRY II

[45 LECTURES]

## **LEARNING OBJECTIVES**

- 1. To study the preparations, reactions and applications of aromatic nitrogen and amino compounds, aromatic aldehydes and ketones, aromatic carboxylic and sulphonic acids with mechanisms of certain reactions.
- 2. To understand stereochemistry including assignment of descriptors to chiral centres and resolution of racemates.
- 3. To logically predict structures of organic compounds and plan multi-step syntheses.
- 4. To understand the concepts of 'clean and green' reactions and techniques that is becoming increasingly significant in making organic synthesis environment friendly.

## UNIT I: Aromatic nitrogen compounds, heterocycles and stereochemistry (15 L)

## 1.1: Aromatic nitro compounds

(3 L)

- **1.1.1: Preparation**: Nitration using mixed acid (mechanism). Preparation of mononitro and dinitro compounds through nitration of benzene, nitrobenzene, toluene, chlorobenzene and anisole.
- **1.1.2: Reactions:** Reduction of aromatic nitro compounds by catalytic hydrogenation, dissolving metal reduction using Fe-HCl, Sn-HCl and Zn- AcOH and partial reduction using NaHS.

## 1.2: Aromatic amino compounds

(2 L)

- **1.2.1: Preparation**: Reduction of nitro compounds, amination of halobenzenes and Hoffmann bromamide reaction.
- **1.2.2: Reactions**: Basicity of aromatic amines, effect of substituents on basicity of aniline, salt formation, N-alkylation and N-acylation.
- 1.3: Aromatic diazonium salts

(2 L)

- **1.3.1: Preparation**: Diazotization of aromatic primary amines (mechanism).
- **1.3.2:** Reactions: (i) Replacement of diazo group by -H, -OH, -CN, Sandmeyer, Gattermann and Gomberg reaction (ii) Azo-coupling reaction with phenols/naphthols and aromatic amines and (iii) Reduction of diazonium salt to aryl hydrazine.

## 1.4: Aromatic heterocycles (4 L)

- **1.4.1:** Electronic structure and aromatic character of furan, thiophene, pyrrole and pyridine.
- **1.4.2:** Reactivity towards electrophilic substitution on the basis of stability of intermediates.
- **1.4.3:** Comparison of basicity of pyrrole, pyridine and piperidine.

## 1.5: Stereochemistry (4 L)

- **1.5.1:** Assigning stereodescriptors to chiral centres: Cahn-Ingold-Prelog (CIP) Rules of assigning absolute configuration (R and S) to stereogenic centres. Assigning absolute configuration to molecules having maximum two chiral carbon atoms.
- **1.5.2:** E and Z stereodescriptors to geometrical isomers.
- **1.5.3:** Chemical Resolution of enantiomers.

## UNIT II: Aromatic carbonyl and acidic compounds, structure determination and multi-step syntheses (15 L)

## 2.1: Aromatic carbonyl compounds (6 L)

- **2.1.1:** Preparation of aromatic aldehydes: Gattermann-Koch reaction, Gattermann reaction, Vilsmeier-Haack reaction, Reimer-Tiemann reaction (mechanism), oxidation of methyl arenes and Rosenmund reduction.
- **2.1.2: Preparation of aromatic ketones:** Friedel-Crafts acylation using acid chloride and acid anhydride (mechanism).
- **2.1.3: Reactions with mechanism**: Knoevenagel, Claisen-Schmidt, Cannizzaro and Reformatsky reactions with applications.

## 2.2: Aromatic carboxylic acids (3 L)

- **2.2.1:** Preparation of mono- and di-carboxylic acids: Side-chain oxidation of alkyl benzenes, reaction of Grignard reagents with solid carbon dioxide, hydrolysis of aryl nitriles and Kolbe-Schmidt reaction.
- **2.2.2:** Reactions: (i) Acidity and effect of substituents on the acidity of benzoic acid (ii) Acid-catalysed esterification, (iii) Conversions to acid chloride, amide and anhydride (iv) Reduction and (v) Decarboxylation.

## 2.3: Aromatic sulfonic acids (2 L)

- **2.3.1: Preparation** of aromatic sulfonic acids: Commonly used sulfonating agents. Sulfonation of benzene (with mechanism) and mono-substituted benzenes.
- **2.3.2: Reactions**: Acidity of arene sulfonic acids. Comparative acidity of carboxylic acids and sulfonic acids, salt formation, desulfonation and Ipso substitution. SO<sub>3</sub>H as a solubilizing and blocking group, preparation of sulfonate esters.

## 2.4: Structure Determination and Multistep Syntheses

(4 L)

- **2.4.1:** Structure determination through a series of reactions.
- **2.4.2:** Planning multistep synthesis of polysubstituted benzenes.

## UNIT III: Green Chemistry and Environment friendly techniques

(15 L)

## 3.1: Green Chemistry

(8 L)

- **3.1.1:** Definition, need and importance of Green Chemistry. 12 principles of Green Chemistry with relevant examples, concepts and simple calculations on yield and selectivity, E-factor, atom economy.
- **3.1.2:** Examples of Green Chemistry in Industry : (i) Green Starting Materials (ii) Green Reagents (iii) Green Chemical Solvents (iv) Green Chemical Products (v) Green Catalysts.

## **3.2:** Environment friendly techniques:

(7 L)

- **3.2.1:** The use of Phase Transfer Catalysis and Polymer Support.
- **3.2.2:** Synthesis using microwave and ultrasound.

### REFERENCES

- 1. Organic Synthesis Special Techniques: V.K.Ahluwalia, Renu Aggarwal, Narosa Publication.
- 2. Organic Chemistry, Francis A Carey, Pearson Education, 6th Edition, Special Indian Education, 2008.
- 3. Organic Chemistry, R.T. Morrison and R.N. Boyd, 6th Edition, Pearson Education.
- 4. Organic Chemistry, Finar Vol. I.
- 5. Fundamentals of Organic Chemistry, G. Marc Loudon, 4th Edition, Oxford University Press, 2006.
- 6. Organic Chemistry, L.G. Wade Jr. and M.S. Singh, 6th Edition, Pearson Education, New Delhi, 2008.
- 7. Organic Chemistry, Paula Y. Bruice, Pearson Education, 2008.
- 8. Organic Chemistry, J.G. Smith, 2nd Edition, Special Indian Edition, Tata McGraw Hill, New Delhi, 2008.
- 9. Organic Chemistry, S.H. Pine, McGraw Hill Kogakusha Ltd.
- 10. Organic Chemistry, J. McMurry, 5th Edition, Asian Books Pvt. Ltd., New Delhi, 2000.
- 11. A guide to mechanism in Organic Chemistry, 6th Edition, Peter Sykes, Pearson Education, New Delhi
- 12. Organic Reaction Mechanism, 3<sup>rd</sup> Edition, V.K. Ahluwalia and R.K. Parashara, Narosa Publications.
- 13. Stereochemistry, P.S. Kalsi, New Age International Ltd., 4th Edition, 2006.
- 14. An Introduction to Green Chemistry, V.K. Ahluwalia, Vishal Publishing Co.

CIA I: Short answer questions 20 MARKS

CIA II: MCQ 20 MARKS

## **Template of Question Paper**

## ORGANIC AND INDUSTRIAL CHEMISTRY II

## **OBJECTIVES**

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL MARKS
I	7	7	6	20
II	7	7	6	20
III	6	7	7	20
TOTAL MARKS PER OBJECTIVE	20	21	19	60
% WEIGHTAGE	33	35	32	100

## **END SEMESTER PAPER PATTERN:**

Total Marks: 60 Maximum Time: 2 hours

Total number of questions: 3 [all compulsory] of 20 marks each.

1 question per unit.

Questions set out of 30 marks [50% internal choice].

Sub questions will not exceed 5 marks.

**COURSE: S.CHE.4.03** 

## PRACTICAL CHEMISTRY

## **LEARNING OBJECTIVES:**

1. To learn to perform experiments that have specific aims with correct techniques.

**Course No.: S.CHE.4.PR** 

- 2. To develop skills of observation, recording and analysing data.
- 3. To learn to present the experimental work in a systematic manner.

## **SEMESTER IV: COURSE 1**

Instrumentation Commercial Analysis

## **SEMESTER IV: COURSE 2**

Gravimetric estimation Volumetric estimation

## **SEMESTER IV: COURSE 3**

**Organic Spotting** 

## **COURSE I:**

1. **POTENTIOMETRY**: Determination of E cell, free energy and equilibrium constant for a cell having cell reaction :  $Ag + Cu \rightarrow Ag + Cu$ 

## 2. pH METRY:

pH metric titration of weak acid versus strong base and to determine pKa value.

## **3.CONDUCTOMETRY:**

Conductometric titration of a mixture of a strong and weak acid versus strong base.

## 4. CONDUCTOMETRY:

Verification of Ostwald's dilution law for weak electrolyte (Acetic acid).

## 5. COLORIMETRY:

Determination of  $\lambda_{max}$  for potassium permanganate solution using photometer, determination of unknown concentration by calibration curve method.

## 6. COMMERCIAL ANALYSIS:

Assay of commercial sample of aspirin using phenol red indicator.

### **COURSE II**

## 1. VOLUMETRIC ESTIMATION:

- a) Iodometry and Iodimetry:
- (i) Estimation of tincture iodine.
- (ii) Estimation of Cu<sup>2+</sup>
- b) Complexometry: estimation of Mg<sup>2+</sup>/Zn<sup>2+</sup>, Cu<sup>2+</sup> using EDTA
- c) Estimation of Fe<sup>3+</sup> using Internal Indicator.

## 2. GRAVIMETRIC ESTIMATION:

- a) Ba<sup>2+</sup> as BaSO<sub>4</sub>
- b) Ba<sup>2+</sup> as BaCrO<sub>4</sub>
- c)  $Fe^{3+}$  as  $Fe_2O_3$
- d) Ni<sup>2+</sup> as Ni-DMG

## **COURSE III**

## **ORGANIC SPOTTING**

**Identification of an Organic Compound:** The identification should be done through: preliminary tests, solubility, element detection, functional group tests, physical constant determination. The analysis should be done by micro-scale techniques. For the identification of an organic compound about 500mg of any compound with not more than two functional/neutral groups be given belonging to the following categories: Acids (carboxylic acids/sulphonic), phenols, aldehydes/ketones, alcohols, esters, amines (primary, secondary and tertiary), carbohydrates, hydrocarbons, halo/nitro hydrocarbons.

Note: A minimum of 12 compounds be given for the identification: at least one from each of the categories mentioned above.

## **CIA AND END SEMESTER PRACTICAL EXAMINATION**

CIA: 20 MARKS PER COURSE PER SEMESTER: Total: 60 MARKS

**COURSE 4.01:** 15 MARKS oral presentation on instrumentation 5 MARKS: journal

**COURSE 4.0 2:** 15 MARKS: exercise to test a quantitative practical skill 5 MARKS: journal

**COURSE 4.03:** 15 MARKS: exercise to test a qualitative practical skill 5 MARKS: journal

**END SEMESTER EXAMINATION**: 30 MARKS PER COURSE Total: **90 MARKS** 

The practical exam will be conducted for 3 sessions (one per course) of 3 hours duration each.

Course 4.01: 25 Marks and 5 Marks written test

Course 4.02: 25 Marks and 5 Marks written test

Course 4.03: 25 Marks and 5 Marks written test

Batch Size: Maximum 20 students per batch.



# St. Xavier's College – Autonomous Mumbai Syllabus for 5<sup>th</sup> Semester Course in Chemistry (June 2014 onwards)

Contents: Theory Syllabus for Courses:

S.CHE.5.01 - SPECTROSCOPY, MOLECULAR & NUCLEAR DYNAMICS

S.CHE.5.02 - CHEMICAL BONDING AND CO-ORDINATION CHEMISTRY

S.CHE.5.03 - STEREOCHEMISTRY AND NATURAL PRODUCTS

S.CHE.5.04 - GENERAL ANALYTICAL CHEMISTRY

S.CHE.5.AC – INTRODUCTION TO NEUROSCIENCE

Practical Course Syllabus for S.CHE 5 PR AND S.CHE 5.AC. PR

## <u>SEMESTER 5</u> SPECTROSCOPY, MOLECULAR & NUCLEAR DYNAMICS

Course No. S.CHE.5.01 60 Lectures

## **LEARNING OBJECTIVES:**

- a) To encourage students to learn, integrate & analyze the concepts relevant to physical chemistry at the graduation level.
- b) To understand the underlying principles of various types of spectroscopy, the rules governing their transitions & their utility in determination of bond length of diatomic molecules & elucidating structures of molecules.
- c) To acquire knowledge about methods of detection of various ionizing radioactive radiations, various types of nuclear reactions & nuclear reactors.
- d) To understand the basics of quantum chemistry & appreciate the concept of entropy as a probability factor.
- e) To learn about basic laws governing photochemical reactions & understand the basic principles of fluorescence, phosphorescence & chemiluminescence.

## **UNIT I: Spectroscopy**

## 1.1 Molecular Spectroscopy:

15 L

- **1.1.1 Dipole moment:** Polarization of a bond, bond moment, dipole moment and molecular structure.
- **1.1.2 Rotational / Microwave Spectroscopy:** Rotational spectrum of a diatomic molecule, rigid rotor, moment of inertia, energy levels, limitations of rotational spectra, selection rule, nature of spectrum, determination of inter nuclear distance and isotopic shift.
- **1.1.3 Vibrational (IR) spectroscopy:** Vibrational motion, degrees of freedom, modes of vibration, vibrational spectrum of a diatomic molecule, simple harmonic oscillator, energy levels, zero point energy, conditions for obtaining vibrational spectrum, selection rule, nature of spectrum. Anharmonic oscillator: energy levels, selection rule, fundamental band, overtones.
- **1.1.4 Vibration-Rotation spectroscopy of diatomic molecules:** Vibrating rotor, energy levels, selection rule, nature of spectrum, R and P branches, applications of vibration-rotation spectrum: (i) Force constant, determination and significance (ii) Determination of internuclear distance, isotopic shift. Introduction to infrared spectra of simple molecules like H<sub>2</sub>O and CO<sub>2</sub>.
- **1.1.5 Raman Spectroscopy:** Scattering of electromagnetic radiation, Rayleigh scattering, Raman scattering, nature of Raman spectrum, Stoke's lines, anti-Stoke's lines, Raman shift, quantum theory of Raman scattering, comparative study of IR and Raman spectra, rule of mutual exclusion (example of CO<sub>2</sub> molecule).

### **UNIT II**

## 2.1. Nuclear Magnetic Resonance Spectroscopy

7 L

- **2.1.1** Nuclear spin, magnetic moment, nuclear 'g' factor, energy levels, Larmor precession. Relaxation processes in NMR (spin-spin relaxation and spin-lattice relaxation),
- **2.1.2** NMR spectrometer, chemical shift, shielding and de-shielding of protons, low resolution NMR spectrum of methanol and ethanol, fine structure of NMR nuclear spin-spin interaction with reference to methanol and ethanol.

## **2.2 Electron Spin Resonance Spectroscopy** (introductory concepts only)

3 L

- **2.2.1** Derivative curves & g-values, Hyperfine splitting with respect to methyl radical and benzene radical.
- 2.2.2 Applications of ESR Spectroscopy

## 2.3 Mass Spectrometry

5 L

- **2.3.1** Basic Principles of mass spectrometry, Molecular ion peak, base peak, metastable peak & their uses, nitrogen rule, fragmentation.
- **2.3.2** Instrumentation, determination of molecular formulae with example, mass spectrum of simple organic compounds eg alkanes.

(Numerical problems expected in the above topics)

## **UNIT-III: Molecular & Nuclear dynamics**

## 3.1 Nuclear Chemistry

15 L

- **3.1.1** Types of nuclear radiations and their characteristics, behaviour of ion-pairs in electric field, detection and measurement of nuclear radiations using G.M. counter and scintillation counter.
- 3.1.2 Kinetics of radioactive decay, units of radioactivity (Curie, Becquerel, Rutherford),
- **3.1.3** Radioactive equilibrium (secular and transient) Determination of radioactive constants for radio-elements having (i) moderate half life (ii) long half life (iii) extremely long or short half life.
- **3.1.4** Use of radioisotopes as tracers in (i) chemical investigations reaction mechanism determination dating by tritium content and by carbon-14.
- **3.1.5** Nuclear Reactions : nuclear transmutation, artificial radioactivity (suitable examples using different projectiles are expected.), Q-value of nuclear reaction threshold energy.
- **3.1.6** Fissile and fertile material, nuclear fission, chain reaction, factors controlling fission process (multiplication factor and critical size or mass of fissionable material), nuclear power reactor and breeder reactor.
- **3.1.7** Nuclear fusion, characteristics of nuclear fusion, thermonuclear reactions occurring in stellar bodies.

### **UNIT IV:**

## 4.1 Basics of Quantum Chemistry

9 L

- **4.1.1** Classical mechanics, limitations of classical mechanics, Black body radiation, photoelectric effect, Compton Effect.
- **4.1.2** Introduction to quantum theory, Planck's theory of quantization, wave particle dualism, deBroglie equation, Heisenberg's uncertainty principle. Simple numerical problems.
- **4.1.3** Progressive and standing waves, boundary conditions, Schrödinger's time independent wave equation, interpretation and properties of wave function.
- **4.1.4** State function (wave function) and its significance. Concept of operators: definition, addition, subtraction and multiplication of operators, commutative and non-commutative operators, linear operator, position, momentum and energy operators. Eigen function and eigen value, eigen value equation.

Self-study: Students to devise own problems on these concepts

## 4.2 Third Law of Thermodynamics

3 L

- **4.2.1** Entropy & probability: recapitulation
- 4.2.2 Statement of Third Law of Thermodynamics
- **4.2.3** Absolute entropy of solids, liquids & gases.

## 4.3 Photochemistry

3 L

- **4.3.1** Laws of Photochemistry, Jablonski energy level diagram primary & secondary photochemical processes.
- **4.3.2** Radiationless transition internal conversion & intersystem crossing.
- **4.3.3** Radiative transitions fluorescence, relation to structure. Phosphorescence- conditions for phosphorescence emission (spin orbit coupling). Singlet and triplet.
- 4.3.4 Chemiluminiscence.

## Evaluation: One of the two CIA evaluations will be a written assignment

## REFERENCE BOOKS

- 1. P.W. Atkins, The Elements of Physical Chemistry: 4<sup>th</sup> ed. Oxford University Press, 2005
- **2. G.M. Barrow**, Physical Chemistry: 6<sup>th</sup> Ed, Tata McGraw Hill Publishing Co. Ltd., 2008.
- **3. G.K. Vemulapalli,** Physical Chemistry: Prentice Hall of India Pvt. Ltd., (2009).
- **4. G.W. Castellan,** Physical Chemistry: 3<sup>rd</sup> ed., Narosa Publishing House, 2004.
- **5. S. Glasstone,** Text Book of Physical Chemistry, 2<sup>nd</sup> ed, Affiliated East-West press Pvt.Ltd., New Delhi.

- 6. S. Glasstone, Thermodynamics for Chemist: Affiliated East-West Press Pvt. Ltd., New Delhi.
- **7. K.J. Laidler and J.H. Meiser,** Physical Chemistry: 2<sup>nd</sup> ed. CBS (First Indian ed.1999) Publishers and Distributors, New Delhi.
  - 8. Ira N.Levine, Physical Chemistry: 6th ed., Tata McGraw Hill, Inc 2011
- **9. Reisman Arnold,** Phase equilibria –Edited by Ernest M. Loebe, New York AND London Academic Press.
  - 10. F.D. Ferguson and P.K. Jones, Phase Rule: (Bitterworth Publisher).
  - 11. J.N. Murrell and E.A. Boucher, Properties of Liquids and Solution: Wiley, 1982.
  - **12. D.K. Chakravarty,** Adsorption and Catalysis:, Oxford Publishers.
  - 13. D.J. Shaw, Introduction to Colloid and Interface Science: Butterworth and Co. (1981).
  - 14. D.H.Everett, Basic Principles of Colloid Science: Royal Society of Chemistry, (1988).
- **15. Nakamura A. and M.Tsutsui,** Principles and Applications of Homogeneous Catalysis: Wiley, (1980)
- **16. Thomas J.M., and Thomas W.J.,** Introduction to Principles of Heterogeneous Catalysis: VCH Publishers, New York, 2008.
- **17. C.N. Banwell**, Fundamentals of Molecular Spectroscopy, 5<sup>th</sup> ed. .Tata McGraw Hill Publishing Co. Ltd, New Delhi,
- **18. Friedlander, Kennedy and Joseph W.,** Nuclear and Radiochemistry –John Wiley & sons, NewYork 1955.
- **19. Arnikar H.J.,** Essentials of Nuclear Chemistry: 4<sup>th</sup> ed, New Age International Ltd., Publishers, New Delhi.1955
  - 20. Maheshwar Sharon and Madhuri Sharon, Nuclear Chemistry: Ane Books Pvt ,ltd 2009.
  - **21. K.J. Laidler**, Chemical Kinetics –3<sup>rd</sup> edn..., New York, Harper & Row, 1987.
  - 22. Masel R.I, Chemical Kinetics and Catalysis, John Wiley Hoboken (2001).
  - 23 Donald A. McQuarrie, Quantum Chemistry: Viva Books Pvt Ltd, 2003.
- **24. R.K.Prasad,** Quantum Chemistry: 3<sup>rd</sup> ed., New Age International (p) Ltd., Publishers, New Delhi.2000.
- **25. Fred W. Billmeyer,** A Text Book of Polymer Science : 3<sup>rd</sup> ed., John Wiley & Sons.Singapore, 1984
  - **26 Bhatnagar M.S:** Textbook of Polymers (Vol 1 3)., S. Chand & Co. Ltd, New Delhi (2010).
  - 27. Samuel Glasstone, An Introduction to Electrochemistry –Affiliated East-West Press.
- **28.** J. O'M Bokris and A.K.N. Reddy, Modern Electrochemistry:– Gamboa-Aldeco, Maria, Vol 2A, 2<sup>nd</sup> ed, 1<sup>st</sup> Indian reprint, Springer, (2006).

- **29. D.R.Crow**, Principles and Applications of Electrochemistry : 4<sup>th</sup> ed., Boka Ralon, Chapman & Hall, London, (1994)
- **30. D.K. Chakravarty,** Solid State Chemistry, New Age International (p) Ltd., Publishers, New Delhi. 1996
- **31. J.A.K. Tareen and T.R.N. Kutty.** A Basic Course in Crystallography, Unversity Press, (2001)
- **32.** C.N.R. Rao and J. Gopalakrishnan, New Directions in Solid State Chemistry: 2<sup>nd</sup> ed., Cambridge University Pres (1989).
- 33. P.S. Sindhu, Molecular Spectroscopy: Tata McGrow Hill Co. Ltd., New Delhi (1993).
- **34. G. Chatwal and S. Anand**, Instrumental Methods of Chemical Analysis: 5<sup>th</sup> ed., Himalaya Publication. 2002
- **35. S.R.Metz,** 2000 Solved Problems in Physical Chemistry: Tata McGraw Hill Publishers, New Delhi.
- **36 O'M Bockris &. S.N. Srinivasan,** Fuel cells; their electrochemistry, McGraw Hill, New York (1969)
- 37 'Chemical & Electrochemical energy systems' University, Press (India) Ltd.1998.
- **38. Godfrey Boyle**, 'Renewable Energy': Publisher: OUP Oxford; 2<sup>nd</sup> edition(March 2004)
- **39. S.N. Lee & James G. Spergit,** Handbook of alternative fuel technologies, CRC Press.
- **40. C.Dubey**, Textbbook of Biotechnology. S. Chand, New Delhi.
- **41. Donald L. Klass**, Biomas for Renewable Energy, fuels & Chemicals, Academic Press, London, UK.1998
- **42. K.L. Kapoor**, A Textbook of Physical Chemistry, (Vol 1 5) Macmillan India Ltd, 2008
- **43. C N Banwell & E.M Mc Cash,** Fundamentals of Molecular Spectroscopy: 4<sup>th</sup> ed. Tata Mc Graw Hill Publication. 1995
- **44.** William Kemp, Organic Spectroscopy: MacMillan Publisher, London, 1975

## SEMESTER 5 Course No: S.CHE 5.02 CHEMICAL BONDING AND CO-ORDINATION CHEMISTRY 60 Lectures

## **Learning Objectives:**

- 1.To encourage students to analyze and integrate concepts relevant to graduate level inorganic chemistry
- 2 To understand the bond formation of compounds with special reference to MOT and CFT
- 3 To build on basic concepts of Coordination Chemistry with reference to planar, tetrahedral and octahedral complexes.
- 4 To study Electronic Spectra of Polyelectronic atoms.

## **UNIT I: Chemical Bonding**

## 1.1. Molecular symmetry

7 L

- **1.1.1** Introduction and Importance
- **1.1.2** Symmetry elements and symmetry operations
- **1.1.3** Concept of a Point Group with illustrations using the following point groups: (i)  $C_{\infty v}$  (HCl), (ii)  $D_{\infty h}$  (H<sub>2</sub>), (iii)  $C_{2v}$  (H<sub>2</sub>O), (iv)  $C_{3v}$  (NH<sub>3</sub>), (v)  $C_{2h}$  (transdichloroethylene), and (vi)  $D_{3h}$  (BCl<sub>3</sub>)

Self Study: Molecular symmetry for MX<sub>3</sub>: planar and pyramidal;  $D_{4h}$  and  $C_4$ 

## 1.2 Molecular Orbital Theory for polyatomic species

5 L

- **1.2.1** Simple triatomic species H<sub>3</sub><sup>+</sup> and H<sub>3</sub> (correlation between bond angle and molecular orbitals with reference to Walsh diagram).
- **1.2.2** Other molecules (considering only  $\sigma$  bonding) : (i) BeH<sub>2</sub>, (ii) H<sub>2</sub>O, (iii) NH<sub>3</sub>, and (iv) CH<sub>4</sub> (with reference to Walsh diagram).

Self Study: Molecular orbital diagram for CO<sub>2</sub>

## 1.3 Metallic Bond 3 L

- **1.3.1** Band theory
- **1.3.2** Explanation of electrical properties of conductors, insulators and semiconductors (n-and p-types) on the basis of Band theory

## **UNIT II: Inner Transition Elements**

## 2.1 Lanthanide series

11L

- **2.1.1** Chemistry of lanthanides with reference to (i) lanthanide contraction, (ii) oxidation states, (iii) magnetic properties, (iv) colour and spectra (f-f transition spectra), and (v) complex formation (types and stereochemistry of the complexes).
- **2.1.2** Separation of lanthanides by (i) ion-exchange, and (ii) solvent extraction methods.

Self Study: i) Occurrence & extraction of Lanthanides

ii) Application of lanthanides

2.2 Actinide series 4 L

**2.2.1** Chemistry of Uranium and Plutonium with reference to occurrence, extraction extraction method), properties and applications.

Self Study: i) Applications of actinides

ii) Comparative chemistry of lanthanides and actinides

### **UNIT III**

## **Co-ordination Chemistry**

## 3.1 Crystal field theory (CFT)

8 L

- **3.1.1** Basic tenets of Crystal Field Theory and effect of Crystal Field on central metal valence orbitals
- **3.1.2** Splitting of d orbitals in octahedral, tetrahedral and square planar complexes and Jahn Teller Effect
- **3.1.3** Crystal field splitting energy  $(10D_q/\Delta_o)$  for octahedral complexes and factors affecting the magnitude of  $\Delta_o$ .
- **3.1.4** Crystal field stabilization energy (CFSE), calculation of CFSE for octahedral and tetrahedral complexes with d<sup>1</sup> to d<sup>10</sup> metal ion configurations, high-spin and low-spin complexes.
- 3.1.5 Effect of crystal field splitting on (i) Ionic radius, and (ii) Lattice energy.
- **3.1.6** Experimental evidence for co-valence in co-ordination compounds:
  - (i) ESR spectrum of [IrCl<sub>6</sub>]<sup>2</sup>-.
  - (ii) NMR spectrum of tris(acetylacetonato)vanadium(III) complex,
  - (iii) Intensities of d-d transitions, and (iv) Nephelauxetic effect.

Self Study: Merits and Demerits of CFT.

## 3.2 Molecular orbital theory (MOT) of coordination complexes. 4 L

- **3.2.1.** Application to octahedral complexes in case of (i)  $[Ti(H_2O)_6]^{3+}$  (ii) Fluoro complexes of Fe (II) and Co (III) (iii) Cyano complexes of (Fe (III) and ammino complexes of Co (III).
  - *Self Study*: Molecular orbital diagram for Fluoro complexes of Fe(III) and Cyano Complexes of Fe (II)
- **3.2.2.** Effect of pi-bonding on ligand field splitting parameter in M $\rightarrow$ L  $\pi$  and L $\rightarrow$ M  $\pi$  interactions.

## 3.3 Stability of octahedral complexes

3 L

- **3.3.1.** Thermodynamic stability and kinetic stability of complexes with examples.
- **3.3.2.**Stability constants: stepwise and overall constants and their inter-relationship.
- **3.3.3.** Factors affecting thermodynamic stability

Self Study: Method of determination of stability constants

## **UNIT 1V: Spectra and Substitution Reactions**

## 4.1 Electronic states and terms of polyelectronic atoms

4 L

- **4.1.1** Introduction: electronic configuration and electronic states, Term symbols, coupling of spin momenta (M<sub>S</sub>), orbital momenta (M<sub>L</sub>) and spin orbit coupling or Russell-Saunders coupling.
- **4.1.2** Determination of Terms for p.p and  $p^2$  electronic configuration (as in a carbon atom). Hund's rule
- **4.1.3.** Terms and micro-states for transition metal atoms/ions

## 4.2 Electronic Spectra

5 L

- **4.2.1** Types of electronic transitions like intra-ligand transitions, charge transfer transitions and intra-metal transitions (d-d or ligand field transitions for transition metals).
- **4.2.2** Rules for electronic transitions: Spin and Orbital or Laporte selection rules
- **4.2.3** Splitting of Terms in weak crystal field, the Hole Formalism.
- **4.2.4** Orgel Diagrams for D Terms (i.e  $d^1$ ,  $d^4$ ,  $d^6$ ,  $d^9$  electronic configurations) and their use in interpretation of visible electronic absorption spectra of these configurations.

Self Study: Application of Electronic spectra

## 4.3. Substitution reactions in octahedral complexes

6 L

- **4.3.1** Introduction, types of reactions in complexes
- **4.3.2** Ligand substitution reactions: basic mechanism
- 4.3.3 Inert and labile complexes and electronic configurations and lability of complexes
- **4.3.4** Acid hydrolysis, base hydrolysis and anation reactions.

## CIA: One of the two CIAs will be a MCQ quiz

### REFERENCE BOOKS

- 1. **James E. Huheey,** Inorganic Chemistry-Principles of structure and reactivity, Harper & Row Publishers. London 1993
- 2. **D. F. Shriver and P.W. Atkins,** Inorganic Chemistry, 3<sup>rd</sup> edition., Oxford University Press. 1999
- 3. **F. A. Cotton, G. Wilkinson, C. Murillo and M. Bochmann,** Advanced Inorganic Chemistry, 6th ed., John Wiley, New York, 1999.

- 4. **J. D. Lee,** Concise Inorganic Chemistry, 5<sup>th</sup> ed., Blackwell Science Ltd., 2005.
- 5. Gary Wulfsberg, Inorganic Chemistry; Viva Books P A Ltd. New Delhi; 2010.
- 6. **Gary L. Miessler and Donald A. Tarr**, Inorganic Chemisty, 3<sup>rd</sup> edition, Pearson Education Inc. 2004.
- 7. H.H. Jaffee and M. Orchin, Symmetry in Chemistry, New Delhi, Wiley Eastern, 1965
- 8. **J. M. Hollas,** Symmetry in Chemiostry, Chapman and Hall., NY, 1972
- 9. **F.A. Cotton,** Chemical Application of Group Theory, 2<sup>nd</sup> edition, Wiley Eastern Ltd., New Delhi, 1976.
- 10. **C.J. Ballhausen and H.B. Gray,** Molecular Orbital Theory, McGraw-Hill, New York, 1965
- 11. **R. L. Dekock and H. B. Gray,** Chemical Structure and Bonding, The Benjamin Cummins Publishing Company, 1980
- 12. **A. R. West,** Solid State Chemistry and its Applications, John Wiley & Sons, Singapore (2008)
- 13. **Lesley Smart and Elaine Moore,** Solid State Chemistry Introduction, 2<sup>nd</sup> Edition, Nelson Thornes Ltd., UK, 1996
- 14. **Ulrich Muller,** Inorganic structural Chemistry, 2<sup>nd</sup> edition, John Wiley and Sons. Chichester, 1993
- 15. **R.N. Kutty and J. A. K. Tareen,** Fundamentals of Crystal Chemistry, Universities Press (India) Ltd.
- 16. **H. V. Keer,** Principles of the Solid State, New Age International, 1993.
- 17. **D. K. Chakraborty**, Solid State Chemistry, New Age International Publishers, 1996.
- 18. N. N. Greenwood and A. Earnshaw, Chemistry of Elements, Pergamon, New York, 1984
- 19. H. Sisler, Chemistry in Non-aqueous Solvents, Reinhold Publ., New York, 1961
- 20. J. J. Lagowski, The Chemistry of Non-aqueous Solvents. Academic press, New York and London
- 21. **C. M. Day & J. Selbin,** Theoretical Inorganic Chemistry, 2<sup>nd</sup> ed, Affiliated East West Press Pvt. Ltd., 1971
- 22. L.E. Orgel, An Introduction to Ligand Field Theory, Meuthen & Co. Ltd., London, 1960
- 23. **F. Basolo and R. G. Pearson,** Mechanism of Inorganic Reactions, 2<sup>nd</sup> ed, Wiley, New York, 1973

## <u>SEMESTER 5</u> STEREOCHEMISTRY AND NATURAL PRODUCTS Course: No. S.CHE.5.03 60 Lectures

## **Learning Objectives**

- 1. To consolidate the students' understanding of the stereochemistry of molecules and reactions
- 2. To investigate reaction mechanism
- 3. To give the students an overview of biomolecules
- 4. To enable students to apply their knowledge of spectroscopy in the determination of the structure of simple organic molecules
- 5. To study mechanisms involved in some name reactions
- 6. To give the students a knowledge of some reagents and catalysts in organic syntheses and an introduction to the concept of retrosynthesis
- 7. To give the students an overview of polymers

## UNIT I

## 1. 1. Stereochemistry

15 L

- **1.1.1. Configurational descriptors:** Compounds with two stereogenic centres represented in Fischer and Sawhorse projection formulae. Geometrical isomers.
- **1.1.2 Elements of symmetry:** Mirror plane, centre (inversion centre), rotation-reflection (alternating) axis.
- **1.1.3 Molecular chirality:** Compounds without stereogenic centres but with chiral axis: cummulenes, spirans and biphenyls; and with chiral planes: cyclophanes and ansa compounds.
- **1.1.4. Conformational analysis of cyclohexane:** Angle, eclipsing and transannular strain. Mono- and di-alkyl cyclohexanes and their relative stabilities.
- **1.1.5. Stereoselectivity and stereospecificity**: Idea of enantioselectivity (*ee*) and diastereoselectivity (*de*). Topicity enantiotopic and diastereotopic atoms, groups and faces.

## 1.1.6. Stereochemistry and mechanism of reactions:

- a) Substitution reactions  $-S_N1$ ,  $S_N2$ ,  $S_Ni$ .
- b) Elimination reactions E1 and E2.
- c) Addition reactions to olefins i) catalytic hydrogenation ii) bromination iii) synhydroxylation with OsO<sub>4</sub> and KMnO<sub>4</sub>.

## **UNIT II**

## 1.2. Mechanism of organic reactions

15 L

- **1.2.1 Investigation of reaction mechanisms:** Product analysis including crossover products, trapping of intermediates, isotopic labeling; kinetic and stereochemical evidence.
- **1.2.2 Thermodynamic and kinetic control of organic reactions:** Concept with mechanisms of the following reactions: Addition of HX to butadiene; sulfonation of naphthalene. Nucleophilicity/electrophilicity v/s Basicity/acidity.

## 1.2.3 Mechanism of reactions of carbonyl compounds with nucleophiles:

- a) Formation of acetals from aldehydes and ketones.
- b) Reaction of aldehydes and ketones with primary and secondary amines.
- c) Acyl nucleophilic substitution (tetrahedral mechanism): Acid catalysed esterification of carboxylic acids and base promoted hydrolysis of esters.
- 1.2.4 Effect of neighbouring group participation (NGP) on organic reactions.

## **UNIT III: Natural Products**

15L

**2.1. Introduction:** Primary and secondary metabolites. Introduction to natural products with respect to sources and classes.

### 2.2 Carbohydrates:

- **2.2.1 Introduction:** Classification, Sources. Reducing and non-reducing sugars. DL notation.
- **2.2.2 Structures of monosaccharides:** Fischer projection (4-6 carbon monosaccharides) and Haworth formula Furanose and pyranose forms of pentoses and hexoses. Interconversion: Open and Haworth forms of monosaccharides with 5 and 6 carbons. Chair conformation with stereochemistry of D-glucose and D-fructose. Stability of chair forms of D-glucose.
- **2.2.3 Determination of open chain configuration:** D-glucose assuming the configuration of D-arabinose; D-fructose assuming the configuration of D-glucose.
- **2.2.4 Stereoisomers of monosaccharides:** Enantiomers and diastereomers of glucose, epimers. Mutarotation (with mechanism) in D-glucose, anomers.
- **2.2.5** Chain lengthening and shortening reactions: Modified Kiliani-Fischer synthesis. Wohl method.

- **2.2.6. Reactions of D-glucose and D-fructose:** (a) osazone formation (b) reduction with H<sub>2</sub>/Ni, NaBH<sub>4</sub> (c) oxidation by bromine water, HNO<sub>3</sub> and HIO<sub>4</sub> (d) conversion of D-glucose to D-fructose (e) acetylation (f) methylation [e and f with cyclic pyranose form]
- **2.2.7 Glycosides:** General structure (example: indican)

UNIT IV 15 L

### 2.4 Amino acids and Proteins:

- **2.4.1** Amino acids: classification, synthesis of  $\alpha$ -amino acids and their detection.
- **2.4.2 Peptide:** stereochemistry of peptide bond, synthesis of peptides by solution (Bergman method) and solid phase (Merrifield method) techniques.
- **2.4.3 Proteins**: classification, properties, primary and secondary structure, denaturation and renaturation.
- **2.4.4.** Separation and purification of proteins: dialysis, gel filtration, electrophoresis.
- **2.4.5.** Catabolism of amino acids: Transamination, oxidative deamination, decarboxylation. The urea cycle and other possibilities of detoxification of ammonia.

## 2.5 Nucleic Acids

- **2.5.1** Controlled hydrolysis of nucleic acids. Bases and sugars in nucleic acids.
- 2.5.2 Structures of nucleosides and nucleotides.
- **2.5.3.** Structures of DNA and RNA.
- **2.5.4** Biosynthesis of DNA: Replication, Genetic code mutations and mutants. DNA repair.
- **2.5.5**.DNA sequencing and PCR, recombinant DNA technology, DNA polymorphism.
- **2.5.6** Biosynthesis of mRNA: Transcription. Biosynthesis of proteins

## 2.6 Alkaloids and Terpenoids

- **2.6.1** Introduction, functions of alkaloids and terpenoids.
- **2.6.2** Structure elucidation, synthesis and biological properties of nicotine and citral.
- **CIA I:** Models or 3-D representations of molecules with stereochemistry.

## **Reference Books:**

- (1) **Francis A Carey,** Organic Chemistry, Pearson Education, 7<sup>th</sup> Edition, Tata McGraw Hill, 2008.
- (2) **R.T. Morrison and R.N. Boyd,** Organic Chemistry, 6<sup>th</sup> Edition, Pearson Education.2008
- (3) **G. Marc Loudon**, Fundamentals of Organic Chemistry, , 4<sup>th</sup> Edition, Oxford University Press, 2006.
- (4) **L.G. Wade Jr. and M.S. Singh,** Organic Chemistry, 6<sup>th</sup> Edition, Pearson Education, New Delhi, 2008.
- (5) **Paula Y. Bruice,** Organic Chemistry, 3<sup>rd</sup> ed, Pearson Education, 2007.
- (6) **J.G. Smith,** Organic Chemistry, 2<sup>nd</sup> Edition, Special Indian Edition, Tata McGraw Hill, New Delhi, 2008.
- (7) **S.H. Pine,** Organic Chemistry, 5<sup>th</sup> ed, McGraw Hill Kogakusha Ltd.2007
- (8) **J. McMurry**, Organic Chemistry, 5<sup>th</sup> Edition, Asian Books Pvt. Ltd., New Delhi, 2006.
- (9) **Peter Sykes,** A guide to mechanism in Organic Chemistry, 6<sup>th</sup> Edition, Pearson Education, New Delhi.
- (10) **V.K. Ahluwalia and R.K. Parashar,** Organic Reaction Mechanism, 4<sup>th</sup> ed., Narosa Publications.
- (11) **P.S. Kalsi,** Stereochemistry, conformation and mechanism, 7<sup>th</sup> ed, New Age International Ltd., 2008.
- (12) **E. L. Eliel,** Stereochemistry of Carbon compounds, Tata McGrawHill, New Delhi.
- (13) V.K. Ahluwalia, Textbook of Organic Chemistry, (Vol 1 3), Ane Books Pvt Ltd 2010
- (14) **P.S. Kalsi,** Stereochemistry through solved problems, Wiley Eastern, 1994
- (15) **P.S. Kalsi,** Spectroscopy of Organic compounds, New Age International Ltd, 1995
- (16) **Jagmohan,** Organic Spectroscopy- Principles and Applications- 2<sup>nd</sup> ed., Narosa Publication.2008
- (17) **W. Kemp,** Organic Spectroscopy, , 3<sup>rd</sup> Edition, Palgrave, Indian Edition, 2005.
- (18) **Williams and Fleming,** Spectroscopic methods in Organic Chemistry, 5<sup>th</sup> ed, McGraw Hill 1995
- (19) **B.G. Devis and A.J. Fairbanks,** Carbohydrate Chemistry, Oxford University Press, New Delhi, Indian Edition, 2005.
- (20) **D. Walton and P. Lorimer**, Polymers, Oxford University Press, New Delhi, Indian Edition, 2005.
- (21) V.K. Ahluwalia, Terpenoids, Ane Books Pvt. Ltd., New Delhi, 2009.
- (22) **V.K. Ahluwalia and A. Mishra,** Polymer Science, Ane Books Pvt. Ltd., New Delhi, 2009.
- (23) V.K. Ahluwalia, An introduction to Green Chemistry, Vishal Publishing Co.
- (24) K.S. Tewari, N.K. Vishnoi, Organic Chemistry, Vikas Publications.
- (25) **N.K. Vishoi**, Advanced Practical Organic Chemistry, 2<sup>nd</sup> Edition, Vikas Publications.
- (26) **I.L.Finar,** Organic Chemistry, 6<sup>th</sup> ed Volume 2 Stereochemistry and the Chemistry of Natural Products, Fifth Edition, Pearson.
- (27) Satyanarayan Biochemistry
- (28) **Stuart Warren,** Designing Organic Syntheses, Wiley India Pvt. Ltd., 2009.

\*

## SEMESTER 5 Course: No. S.CHE.5.04 GENERAL ANALYTICAL CHEMISTRY 60 Lectures

## **Learning Objectives:**

- 1. To understand sources of errors in measurement
- 2. To promote an understanding about data collection, manipulation and interpretation.
- 3. To expose students to commonly used sampling techniques
- 4. To understand the principles involved in titrimetry
- 5. To introduce students to modern analytical techniques.
- 6. To comprehend the principles and techniques involved in chromatography and solvent extraction.
- 7. To motivate students to solve numerical problems

## **UNIT I: Errors and Treatment of analytical data**

15 L

- **1.1.** Types of errors, determinate and indeterminate errors, minimization of errors, constant and proportionate errors
- **1.2** Accuracy and precision, measures of dispersion and central tendency: mean, median, average deviation, relative average deviation, standard deviation, variance, coefficient of variation.
- **1.3** Distribution of random errors, Gaussian curve, Student's t, confidence limits and confidence interval,
- 1.4. Criteria for rejection of result: 2.5 d rule 4.0 d rule, Q test,
- **1.5**. Testing for significance, null hypothesis, F test,
- **1.6**. Graphical representation of data: method of averages, least squares method.

[Numerical problems expected]

## **UNIT II: Sampling**

15 L

- **2.1** Terms involved in sampling, importance of sampling,
- **2.2**. Sampling techniques, equipments used in sampling of gases.
- **2.3.** Methods and equipments used in sampling of homogeneous and heterogeneous liquids, sampling of static and flowing liquids
- **2.4** Samplers used in sampling of solids, importance of particle size and sample size, Methods of reduction in sample size. Collection, preservation and dissolution of the sample.

## **UNIT III: Titrimetric Analysis**

15 L

- **3.1.** Acid –base titrations: construction of titration curves and choice of indicators in the titration of: (i) strong acid and weak base, (ii) weak acid and weak base (iii) dibasic acid and strong base.
- **3.2**. **Precipitation titrations:** Argentimetric titrations, construction of the titration curves, detection of end point by (i) Mohr's method (ii) Volhard's method (iii) using adsorption indicators, theory and applications.
- **3.3. Complexometric titrations:** General introduction, EDTA titrations, advantages and limitations of EDTA as the titrant, absolute and conditional formation constants of metal- EDTA complexes, construction of titration curves, types of EDTA titrations, methods of increasing the selectivity of EDTA as a titrant, metallochromic indicators, theory and applications.
- **3.4. Redox titrations:** General introduction, theory of redox indicators, construction of the titration curves in the case of (i) Fe (II) vs. Ce(IV) (ii) Fe(II) vs. dichromate. Use of diphenyl amine and ferroin as redox indicators.

## **UNIT IV: Separation Techniques**

15 L

- **4.1 Solvent extraction**: role of complexing agents in solvent extraction , chelation, ion pair formation, solvation, solid phase extraction
- **4.2. Chromatography:** introduction to chromatographic techniques, basic principles, classification of chromatographic techniques.
  - **4.2.1** Planar chromatography: principle, techniques and applications of Paper chromatography and Thin layer chromatography
  - **4.2.2** Electrophoresis, slab electrophoresis,
  - **4.2.3**. Size exclusion chromatography: Principle and applications.
  - **4.2.4.** Ion exchange chromatography: types of ion exchangers, mechanism of ion exchange, selectivity coefficients and separation factors, ion exchange capacity and its determination, factors affecting the separation of ions, applications.

### One of the two CIAs will be an Oral Presentation

## **Reference Books:**

- 1 **D. A. Skoog, D.M.West, F.J.Holler** Fundamantals of Analytical Chemistry, 8<sup>th</sup> ed. Philadelphia, Saunders college Publishing, 1996
- 2 **D. A. Skoog, F.J.Holler, T.A.Nieman,** Principles of Instrumental Analysis, 6<sup>th</sup> ed. Philadelphia, Saunders college Publishing, 1996
- 3 **G.D.Christian,** Analytical Chemistry, 6<sup>th</sup> ed. John Wiley &Sons, Singapore, 2004.
- 4 **J.G.Dick,** Analytical Chemistry, International Student's Edition, McGraw Hill, Kogakusha Limited, New Delhi, 1973.
- 5 **R.A.Dey & D.L.Underwood,** Quantitative Analysis, 6<sup>th</sup> ed. Prentice Hall Of India Pvt. Ltd. New Delhi, 1993.
- 6 **M.Valcarcel,** Principles Of Analytical Chemistry, Springer International Edition, Berlin, 2000
- 7 E..Prichard, & V. Barwick, Quality Assurance in Analytical Chemistry, Wiley.
- 8 **S. M. Khopkar,** Basic Concepts of Analytical Chemistry, 3<sup>rd</sup> ed,New Age International Publishers, 2008
- 9 **S. M. Khopkar,** Analytical Chemistry Problems and Solutions, New Age International Publishers, 2002
- 10**A I Vogel,** Textbook of Quantitative Chemical Analysis, 6<sup>th</sup> ed, Pearson Education, 2002
- 11 **Kolthoff and Elving,** Treatise on Analytical Chemistry, Part I Vol 1, Interscience Encyclopedia 1959
- 12 J M Miller, Separation methods in Chemical Analysis, John Wiley, 1975
- 13 J A Dean, Chemical Separation Methods, 1969
- 14 R.D. Braun, Introduction to Instrumental methods of Analysis, McGraw Hill, 1987
- 15 **G R Chatwal and S K Anand**: Instrumental methods of Chemical Analysis, 5<sup>th</sup> ed, Himalaya Publishing House, 2002
- 16**H H Willard, L L Merritt and J A Dean**; Instrumental methods of Analysis, 7<sup>th</sup> ed CBS Publishers, 1986

\*

## TYBSc SYLLABUS UNDER AUTONOMY CHEMISTRY

Semester 5 Course No: S.CHE.PR.5

## **Course 5.01: Physical Chemistry**

## **Instrumental Experiments**

## **POTENTIOMETRY**

- 1. To determine the pK<sub>a</sub> value of a given weak monobasic acid (CH<sub>3</sub>COOH) by e.m.f. measurements using Quinhydrone electrode.
- 2. To determine solubility product and solubility of silver chloride potentiometrically using chemical cell.
- 3. To determine solubility product and solubility of silver chloride potentiometrically using concentration cell.
- 4. To determine electrode potential of saturated calomel electrode at room temperature and using this value to determine standard potential of Ag<sup>+</sup> | Ag electrode.
- 5. To determine the amount of Fe (II) and formal redox potential in the given solution by potentiometric titration against a standard solution of potassium dichromate.

## **CONDUCTOMETRY**

- 6. To determine the relative strength of monochloroacetic acid and acetic acid conductometrically.
- 7. To determine the strength of a given dibasic acid by conductometric titration.

## **POLARIMETRY**

8. To determine the specific rotation of glucose / cane sugar.

## **SPECTROPHOTOMETRY**

9. To verify Beer-Lambert's law using potassium dichromate / potassium permanganate solution, & hence determine its molar absorptivity.

## pH METRY

10. To determine the acidic and basic dissociation constants of an amino acid and its isoelectric point.

# **Course 5.02: Inorganic Chemistry**

# 1. Commercial Analysis

- (i) Analysis of talcum powder for magnesium content.
- (ii) Analysis of calcium tablet.
- (iii) Analysis of boric acid for percentage purity.

# 2. Inorganic Preparations

- (i) Tris-(ethylenediamine)nickel(II)thiosulphate.
- (ii) Bis-(acetylacetonato) copper(II)

# 3. Titrimetric analysis

- (i) Determination of metal content in Tris(ethylenediamine)nickel(II)thiosulphate.
- (ii) Determination of metal content in Bis(acetylacetonato) copper(II).

# Course 5.03: Organic Chemistry

# [A] Organic Separation:

**Separation of a binary mixture:** Type of mixture, Separation and identification (**microscale**) of both components through systematic scheme of identification.

Type: Solid + Solid, (No carbohydrates to be given).

Mass of solid: ~ 3-4g,

# [B] Preparation of Organic compounds:

Preparation of Organic compound as per the procedure given. Measuring the mass of crude, purification of the separated product by crystallization and recording of the m.p.

Quantity of reactant to be given: 1g.

- (1) 2-Naphthol → Methyl ether (using dimethyl sulphate)
- (2) Aniline/p-toluidine → Schiff base with benzaldehyde
- (3) Hydroquinone/2-naphthol → Acetate
- (4) Cyclohexanone  $\rightarrow$  oxime

**Note:** A minimum 6 mixtures should be covered in the semester.

# **Course 5.04: Analytical Chemistry**

# **Non-Instrumental Experiments**

- 1. Estimation of persulphate in the given sample by the method of back titration.
- 2. Determination of the calcium and magnesium content of a Dolomite sample.
- **3.** Determination of glucose content of a honey sample by Willstatter's method.
- 4. Determination of Vitamin C by titration with potassium bromate.
- 5. Determination of dissolved oxygen in the given water sample.
- 6. Determination of Iodine value by Wij's method for the given oil sample.
- 7. Separation of pigments of sketch pen ink.
- 8. Thin layer chromatographic separation of organic compound.
- 9. Chemical Oxygen Demand (COD) of water sample.
- 10. Determination of salinity of the given water sample.

#### References:

- 1. O.P Pandey, D. N. Bajpai and S. Giri, Practical Chemistry, Delhi: S. Chand, 2008.
- **2. V. D.Athawale and P. Mathur,** Experimental Physical Chemistry: New Age International. 2008

# **❖ CIA AND END SEMESTER PRACTICAL EXAMINATION**

**Course 1**: Physical Chemistry – Instrumental Experiment.

**Course 2:** Inorganic Chemistry – Inorganic Preparation and Estimation.

**Course 3:** Organic Chemistry – Separation and Identification of solid-solid mixture.

**Course 4:** Analytical Chemistry – Non-instrumental Experiment.

**Journal**: 5 marks per course.

**CIA:** 15 marks per course.

**Duration**: 4 periods to be conducted during regular practicals by the Faculty-in- charge.

One or more practical skills will be tested in the CIA.

**End Semester Examination**: 30 marks per course. This includes a 5 mark viva-voce based on the theory behind all the experiments conducted per course.

There will be an External Examiner and an Internal Examiner responsible for two courses each.

**Duration**: 3½ hrs per course.

**Batch size**: Max 20 students per batch for courses 2 and 3 and 10 students per batch for courses 1 and 4 (involving instruments).

Course No.: S.CHE.5AC.01

**Total Lectures 60** 

# INTRODUCTION TO NEUROSCIENCE FOUR CREDIT COURSE

# **Learning Objectives:**

This course presents current topics in the broad field of neuroscience and is geared to upper level undergraduate students. The course focuses mostly on mammalian and human brains and resembles in content some of what is taught to most medical students. Topics covered include historical foundations of neuroscience, synaptic and neurotransmitter systems, sensory and motor systems, neurocellular anatomy, motivation, mental illness, and cognitive neuroscience topics. In addition to the lectures in class students will be provided with material for a Study Pack.

UNIT I 15 lectures

# 1.1 Central Nervous System

- 1.1.1 Course content, expectations and examinations; Basic Organization of the CNS
- **1.1.2** Autonomic Nervous Systems
- **1.1.3** Diffuse Modular Systems
- 1.1.4 Neurons and Glia; Neuronal Membrane
- 1.1.5 Action Potential

# 1.2 CNS Drugs

- **1.2.1**Classification based on pharmacological actions
- 1.2.2 Anxiolytics: Barbiturates (Phenobarbitone), Benzodiazepines (Alprazolam)
- 1.2.3 Anticonvulsants and Antiepileptics: Oxazolidinediones (Trimethadione),

Hydantoins (Phenytoin)

- **1.2.4** Antischizophrenics: Phenothiazines (Chlorpromazine)
- 1.2.5 Antidepressants: Imipramine, Fluoxetine

UNIT II 15 lectures

#### 2.1 Working of the CNS

- 2.1.1 Synaptic Transmission: Chemical and Electrical
- **2.1.2** Neurotransmitter Systems
- **2.1.3** Chemical Control of the Brain
- 2.1.4 Neurocortical activation during decision making; Free will?
- 2.1.5 Addictions

# 2.2 Cognition

- 2.2.1 Phantom Syndrome and Pain
- 2.2.2 Motivation
- 2.2.3 Consciousness
- 2.2.4 Perception and Attention

UNIT III 15 lectures

- 3.1 Sensory systems and Processes
- **3.1.1** Visual System
- **3.1.2** Auditory System

- 3.1.3 Somato Sensory System
- **3.1.4** Emotions and Mood
- 3.2 Motor Systems
- **3.2.1** Spinal Control of Movement
- **3.2.2** Alpha Motor Neutrons
- 3.2.3 Gamma Motor Neurons
- **3.2.4** Cortical Control of Movement
- **3.2.5** Planning of Movement by the Cerebral Cortex

UNIT IV 15 lectures

- **4.1 Memory Systems**
- **4.1.1** Memory Systems
- **4.1.2** How we learn and Study
- **4.1.3** Sleep Patterns
- **4.1.4** Stress and De-stress

## 4.2 Neuro-diseases and Everyday Life

- **4.2.1** Neuro diseases of Aging
- **4.2.2** Brain fitness to delay aging
- **4.2.3** Genes or Environment?
- 4.2.4 Brain waves and Meditation
- **4.2.5** Sex and the Brain

**Reference Book**: Handouts will be made available containing reference Study Pack material.

**Examinations**: We follow the Bloomberg System of testing knowledge, understanding and application in equal proportion.

<u>CIA I:</u> 20 Marks Maximum- Consists of questions which are multiple choice, matching, true/false, short answer, labeling brain structures.

**CIA II**: 20 Marks Maximum- Short answer questions.

# **End Semester Paper Pattern:**

Total marks: 60 Marks Maximum. Time: 2 hours Total no. of questions: 10 (out of 12) of 6 marks each Questions may be set out of 9 marks [50 % internal choice]

\*

# **Neuroscience Practical Course: S.CHE. PR. 5.AC.**

# **SEMESTER V**

# **Learning Outcomes**

The experiments for this Practical Course are made up of a set of demonstrations of classic and contemporary experiments and concepts from the neurosciences. These experiments will allow the students to experience at first hand a variety of important experimental studies, which will help them understand the design of the study, the data, and the significance of the research. Besides the content material that students will assimilate it is expected that the practical work will develop in them a keen sense of research methodology as well as incite them to do further reading in the area. It is my hope that, though not a requirement, some of the more interested students would also go on to design other similar experiments, thus giving them a real entry into the world of cognition and neuroscience.

## Methodology

The students are expected to read the background theory. After listening to the instructions they will perform the experiment, note down the data, and then proceed to analyze the data. Results, entered in the proper format have to be initialed by the faculty member supervising the experiment.

# **ATTENTION**

Expt 1: Attentional Blink Expt 2: Change Detection

#### **PERCEPTION**

Expt 3: Apparent Motion Expt 4: Garner Interference

## **NEUROCOGNITION**

Expt 5: Brain Asymmetry

Expt 6: Blind Spot

## **SENSORY MEMORY**

Expt 7: Metacontrast Masking

Expt 8: Modality Effect

# SHORT-TERM MEMORY

Expt 9: Brown-Peterson Expt 10: Position Error

# **WORKING MEMORY**

Expt 11: Irrelevant Speech Effect

Expt 12: Memory Span

**Examination:** There will be one CIA of 20 marks and one end semester examination of 25 marks semester. There will be 5 marks for journal. The practical exam will be conducted for 1 session of 2 hours duration.

Reference: Francis, Greg, Ian Neath, Daniel VanHorn, Coglab, Wadsworth, 2008.

\*



# St. Xavier's College – Autonomous Mumbai Syllabus for 6<sup>th</sup> Semester Course in Chemistry (June 2014 onwards)

Contents: Theory Syllabus for Courses:

S.CHE.6.01 - GENERAL PHYSICAL CHEMISTRY

S.CHE.6.02 - SOLID STATE, SOLUTION AND MEDICINAL CHEMISTRY

S.CHE.6.03 - SPECTROMETRIC IDENTIFICATION AND SYNTHETIC CHEMISTRY

S.CHE.6.04 - INSTRUMENTAL METHODS OF ANALYSIS

S.CHE.6.AC - DRUGS AND COLOUR CHEMISTRY

Practical Course Syllabus for S.CHE 6 PR AND S.CHE 6.AC. PR

# SYLLABUS UNDER AUTONOMY CHEMISTRY

SEMESTER 6 Course: No. S.CHE.6.01

## GENERAL PHYSICAL CHEMISTRY

**60 Lectures** 

# **Learning objectives:**

- a) To encourage students to learn, integrate & analyze the concepts relevant to physical chemistry at the graduation level.
- b) To learn the concept of concentration cells & its applications in determination of several constants & parameters.
- c) To understand & appreciate the utility of electrochemistry in providing renewable sources of energy.
- d) To study various aspects of chemical kinetics, catalysis, surface equilibria & phase equilibria.
- e) To learn the utility of several colligative properties in determination of molecular weight of several solutes & state of solutes that are dissolved to form solutions using van't Hoff factor.

#### UNIT - I:

#### 1.1. Electrochemical cells

15 L

- **1.1.1** Lewis concept of Activity and Activity coefficient, Mean ionic activity and mean ionic activity coefficient  $\gamma_{\pm \text{ of}}$  an electrolyte. Variation of mean ionic activity coefficient with concentration, expression for activities of electrolytes of different valence type, ionic strength of a solution, Debye-Hückel limiting law (derivation not expected)
- **1.1.2** Classification of cells: (i) chemical cells without transference (ii) Concentration cells with and without transference (derivations of expression for concentration cell EMF are expected). Origin of liquid-liquid junction potential, and its elimination using a salt bridge.
- 1.1.3 Applications of EMF .measurements in the determination of (i) Mean ionic activity coefficient of an electrolyte (ii) pH of a solution using quinhydrone and glass electrode. (iii) solubility and solubility product of sparingly soluble salts using chemical cell and concentration cell method (iv) determination of liquid-liquid junction potential (v) determination of ionic product of water using chemical cell and concentration cell method.

#### **UNIT II:**

## 2.1 Applied Electrochemistry

7 L

- **2.1.1** Polarization, concentration polarization and its elimination,
- **2.1.2** Decomposition potential, experimental determination of decomposition potential, factors affecting decomposition potential (nature of electrolyte, nature of electrodes and temperature, overvoltage, experimental determination of over-voltage, Tafel's theory

Page 2 of 29

and Tafel's equation for hydrogen overvoltage, simultaneous deposition of metals,

2.1.3 Electroplating --- objectives and process

# 2.2 Renewable Energy Sources

8 L

- **2.2.1** Batteries Secondary cells, Lithium Ion Cell.
- **2.2.2** Fuel Cells--Choice of fuel and oxidant, thermodynamic and kinetic aspect of electrochemical energy transformation, efficiency of fuel cells , Bacon's  $H_2$  and  $O_2$  fuel cell.
- **2.2.3** Solar cells solar energy, photovoltaic effect, semiconductors as solar energy converters, Silicon solar cell.
- **2.2.4** Biomass energy from biomass and its sources, conversion of biomass into energy by alcohol fermentation and anaerobic digestion method.
- **2.2.5** Hydrogen: fuel of the future Production of hydrogen by direct electrolysis of water and. biomass gasification, advantages of hydrogen as a universal energy medium.

#### UNIT - III:

3.1 Colloids 6 L

- **3.1.1** Introduction to colloidal state of matter.
- 3.1.2. Origin of charge on colloidal particles. Concept of electrical double layer, zeta potential, Helmholtz and Stern mode, Electrokinetic phenomena, (i). Electrophoresis (ii). Electro-osmosis (iii) Streaming potential (iv) Sedimentation potential
- **3.1.3** Colloidal electrolytes.
- 3.1.4 Donnan Membrane Equilibrium.
- **3.1.5** Surfactants, micelle formation, applications of surfactants in detergents, food industry, in pesticide formulations.

# 3.2. Surface Chemistry and Catalysis

9 L

- **3.2.1 Adsorption** Physical and Chemical Adsorption, types of adsorption isotherms,
  - Langmuir's adsorption isotherm, (Postulates and derivation expected). B.E.T. equation for multilayer adsorption, (derivation not expected, significance of the terms involved in the equation is expected.), determination of surface area of an adsorbent using B.E.T. equation.
- **3.2.2 Catalysis** Homogeneous and heterogeneous catalysis, catalytic activity and selectivity, promoters, inhibitors, catalyst poisoning and deactivation, TON and TOF (introduction only)
- **3.2.3** Acid-Base catalysis, mechanism and kinetics of acid-base catalyzed reactions, effect of pH on acid-base catalyzed reactions. Mechanics and kinetics of enzyme catalyzed reaction (Michaelis-Menten equation).
- **3.2.4** Kinetics of surface reactions, heterogeneous catalysis)
  - i) unimolecular surface reactions,
  - ii) bimolecular surface reaction (relevant rate expressions expected)

#### **UNIT IV**

#### 4.1. Chemical Kinetics 6 L

**4.1.1** Collision theory of reaction rates. Application of collision theory to (i) Bimolecular reaction (ii) Unimolecular reaction. (Lindemann theory, derivation expected). Merits and drawbacks of collision theory. Activated complex theory of bimolecular reactions, rate constant of bimolecular reaction (derivation not Expression for Expected), comparison of collision theory and activated complex theory.

**4.1.2** Classification of reactions as Slow, Fast and Ultra-fast. Study of kinetics of fast reactions by Stop flow method.

#### 4.2. Colligative Properties of Dilute Solutions

5 L

- **4.2.1** Dilute solution, colligative properties, Raoult's law, relative lowering of vapour pressure.
- **4.2.2** Elevation in boiling point of a solution, thermodynamic derivation relating elevation in the boiling point of a solution and the molar mass of the non-volatile solute.
- **4.2.3** Depression in freezing point of a solution, thermodynamic derivation relating the depression in the freezing point of a solution and the molar mass of the non-volatile solute.
- 4.2.4 Abnormal molar masses of solutes and van't Hoff factor (calculation of Degree of Association and Degree of Dissociation.)

4.3. Phase Rule 4 L

- **4.3.1** Gibb's phase rule and terms involved in the equation.
- **4.3.2** Application of phase rule to TWO component systems, condensed systems, condensed phase rule, eutectic systems (Lead-Silver system), desilverisation of lead.
- Introduction to THREE component systems, explanation of the phase diagram for three liquids forming one immiscible pair.

Evaluation: One of the two CIA evaluations will be an MCQ quiz

# REFERENCE BOOKS

- 1. P.W. Atkins, The Elements of Physical Chemistry: 4<sup>th</sup> ed. Oxford University Press, 2005
  2. G.M. Barrow, Physical Chemistry: 6<sup>th</sup> Ed, Tata McGraw Hill Publishing Co. Ltd., 2008.
  3. G.K. Vemulapalli, Physical Chemistry: Prentice Hall of India Pvt. Ltd., (2009).
  4. G.W. Castellan, Physical Chemistry: 3<sup>th</sup> ed., Narosa Publishing House, 2004.

- **5. S. Glasstone,** Text Book of Physical Chemistry, 2<sup>nd</sup> ed, Affiliated East-West press Pvt.Ltd., New Delhi.
- **6. S. Glasstone**, Thermodynamics for Chemist: Affiliated East-West Press Pvt. Ltd., New Delhi.
- **7. K.J. Laidler and J.H. Meiser,** Physical Chemistry: 2<sup>nd</sup> ed. CBS (First Indian ed.1999) Publishers and Distributors, New Delhi.

- **8. Ira N.Levine,** Physical Chemistry: 6th ed., Tata McGraw Hill, Inc 2011
- 9. Reisman Arnold, Phase equilibria –Edited by Ernest M. Loebe, New York AND London Academic Press.
- **10. F.D. Ferguson and P.K. Jones**, Phase Rule: (Bitterworth Publisher).
- 11. J.N. Murrell and E.A. Boucher, Properties of Liquids and Solution: Wiley, 1982.
- **12. D.K. Chakravarty,** Adsorption and Catalysis:, Oxford Publishers.
- 13. D.J. Shaw, Introduction to Colloid and Interface Science: Butterworth and Co. (1981).
- 14. D.H.Everett, Basic Principles of Colloid Science: Royal Society of Chemistry, (1988).
- 15. Nakamura A. and M.Tsutsui, Principles and Applications of Homogeneous Catalysis Wiley, (1980)
- 16. Thomas J.M., and Thomas W.J., Introduction to Principles of Heterogeneous Catalysis: VCH Publishers, New York, 2008.
- 17. C.N. Banwell , Fundamentals of Molecular Spectroscopy, 5<sup>th</sup> ed. .Tata McGraw Hill Publishing Co. Ltd, New Delhi,
- 18. Friedlander, Kennedy and Joseph W., Nuclear and Radiochemistry –John Wiley & sons, NewYork 1955.
- 19. Arnikar H.J., Essentials of Nuclear Chemistry: 4<sup>th</sup> ed, New Age International Ltd., Publishers, New Delhi. 1955
  - 20. Maheshwar Sharon and Madhuri Sharon, Nuclear Chemistry: Ane Books Pvt ,ltd 2009.
  - **21.K.J. Laidler**, Chemical Kinetics –3<sup>rd</sup> edn.., New York, Harper & Row, 1987.
  - 22. Masel R.I, Chemical Kinetics and Catalysis, John Wiley Hoboken (2001).
- 23 Donald A. McQuarrie, Quantum Chemistry: Viva Books Pvt Ltd, 2003.
  24. R.K.Prasad, Quantum Chemistry: 3<sup>rd</sup> ed., New Age International (p) Ltd., Publishers, New Delhi.2000.
- 25. Fred W. Billmeyer, A Text Book of Polymer Science : 3<sup>rd</sup> ed., John Wiley & Sons.Singapore, 1984
- **26 Bhatnagar M.S:** Textbook of Polymers (Vol 1-3)., S. Chand & Co. Ltd, New Delhi (2010).
  - **27. Samuel Glasstone**, An Introduction to Electrochemistry –Affiliated East-West Press.
- 28. J. O'M Bokris and A.K.N. Reddy, Modern Electrochemistry: Gamboa-Aldeco, Maria, Vol 2A, 2<sup>nd</sup> ed, 1<sup>st</sup> Indian reprint, Springer, (2006).
- **29. D.R.Crow**, Principles and Applications of Electrochemistry : 4<sup>th</sup> ed., Boka Ralon. Chapman & Hall, London, (1994)
- 30. D.K. Chakravarty, Solid State Chemistry, New Age International (p) Ltd., Publishers, New Delhi.1996
- 31. J.A.K. Tareen and T.R.N. Kutty. A Basic Course in Crystallography, University Press, (2001)
- **32. C.N.R. Rao and J. Gopalakrishnan**, New Directions in Solid State Chemistry: 2<sup>nd</sup> ed., Cambridge University Pres (1989).
- 33. P.S. Sindhu, Molecular Spectroscopy: Tata McGrow Hill Co. Ltd., New Delhi (1993).
- **34. G. Chatwal and S. Anand**, Instrumental Methods of Chemical Analysis: 5<sup>th</sup> ed., Himalaya Publication. 2002
- 35. S.R.Metz, 2000 Solved Problems in Physical Chemistry: Tata McGraw Hill Publishers, New Delhi.
- **36 O'M Bockris &. S.N. Srinivasan,** Fuel cells; their electrochemistry, McGraw York (1969)

- 37 'Chemical & Electrochemical energy systems' University, Press (India) Ltd.1998.
   38. Godfrey Boyle, 'Renewable Energy': Publisher: OUP Oxford; 2<sup>nd</sup> edition( March 2004)
- 39. S.N. Lee & James G. Spergit, Handbook of alternative fuel technologies, CRC Press.
- **40. C.Dubey**, Textbbook of Biotechnology. S. Chand, New Delhi.
- 41. Donald L. Klass, Biomas for Renewable Energy, fuels & Chemicals, Academic Press, London, UK.1998
- **42. K.L. Kapoor,** A Textbook of Physical Chemistry, (Vol 1 5) Macmillan India Ltd, 2008
- **43.** C N Banwell & E.M Mc Cash, Fundamentals of Molecular Spectroscopy: 4<sup>th</sup> ed. Tata Mc Graw Hill Publication. 1995

# SEMESTER 6 Course No. S.CHE 6.02

# SOLID STATE, SOLUTION AND MEDICINAL CHEMISTRY

**60 Lectures** 

# **Learning Objectives:**

- 1. To encourage students to analyze and integrate concepts relevant graduate level Inorganic chemistry
- 2 To understand structure of crystalline solids and defects that exists.
- 3 To expose students to concepts in Superconductivity..
- 4. To study aqueous and non-aqueous solvents
- 5. To introduce students to applications in Medicinal Chemistry

## **UNIT I: SOLID STATE CHEMISTRY**

#### 1.1 Structures of solids

10 L

- **1.1.1** Importance of solid state chemistry
- **1.1.2** Crystals: size and shape of crystals, interfacial angles in crystals, symmetry and elements of symmetry in crystals.
- **1.1.3** Designation of planes in crystals: Miller indices.
- **1.1.4** Classification of solids on the basis of bonding
- **1.1.5** Explanation of terms viz. crystal lattice, lattice points, unit cells, and lattice constants.
- **1.1.6** Closest packing of rigid spheres (hcp, ccp) packing density in simple cubic, bcc, fcc and hcp lattices (numerical problems expected).
- **1.1.7** Structures of metallic solids
- **1.1.8** Tetrahedral and octahedral interstitial voids in ccp lattice, tetrahedral holes, limiting radius ratios for different coordination numbers and their significance, calculation of ionic radii and limiting radius ratio for co-ordination number 4.
- **1.1.9** Structures of sodium chloride, cesium chloride and fluorite.
- **1.1.10** Structure of zinc chloride and failure of radius ratio rule (directional bonding), structure of wurtzite.
- **1.1.11** Defects in crystal structures; Effects of Schottky and Frenkel defects.

# 1.2 Superconductivity

5 L

- **1.2.1** Superconductivity, Meissner effect
- 1.2.2 Different superconducting materials viz., conventional superconductors, organic superconductors, alkali metal fullerides  $(A_3C_{60})$  and high temperature superconductors.

Self Study: Applications of superconducting materials.

## UNIT II

# 2.1 Nanomaterials

5 L

**2.1.1** Introduction and Importance of nanomaterials

- **2.1.2** Properties (Comparison between bulk and nanomaterials): (i) Optical properties, (ii) Electrical conductivity, (iii) Melting points, and (iv) Mechanical properties.
- **2.1.3** Forms of nanomaterials : nanofilms, nanolayers, nanotubes, nanowires and nanoparticles
- **2.1.4** Methods of preparation

# 2.2 Organometallic Chemistry

10 L

- **2.2.1** Organometallic compounds of main group elements:
- **2.2.1.1** Introduction, general synthetic methods: i) Oxidative addition, ii) Metal-Metal exchange (Transmetallation), iii) Carbanion- Halide exchange (Metathesis), iv) Metal-Hydrogen exchange, v) Methylene insertion reactions.
- **2.2.1.2** Chemical reactions: i) Reactions with oxygen and halogens, ii) Alkylation and arylation reactions, iii) Reactions with protic reagents, iv) Redistribution reactions, v) Complex formation reactions.
- **2.2.2** Metallocenes: Synthesis, structure and bonding, reactions and applications of Ferrocene.
- **2.2.3** Bonding in Rhenium and Molybdenum halide complexes.
- **2.2.4** Catalysis with reference to: i) Hydrogenation of alkenes (Wilkinson catalyst), ii) Hydroformylation reaction (Roelen catalyst)

#### **UNIT III: SOLUTION CHEMISTRY**

15 L

# 3.1 Acid-base chemistry in aqueous medium

- **3.1.1** Acidity of mono- and polyatomic cations.
- **3.1.2** Basicity of mono- and polyatomic anions (Latimer equation and predominance diagrams).
- **3.1.3** Measure of acidity and basicity: concepts based on electronegativity and thermodynamic aspects (Drago-Wayland equation).

#### 3.3 Chemistry in Non-aqueous solvents

- **3.2.1** Classification of solvents and importance of non-aqueous solvents.
- **3.2.2** Characteristics of study of liquid ammonia, dinitrogentetraoxide and acetic acid as non-aqueous solvents with respect to (i) acid base reactions (ii) redox reactions.

#### **UNIT IV:**

# MEDICINAL CHEMISTRY AND INORGANIC PHARMACEUTICALS 15 L

#### 4.1 Bioligands in biocoordination chemistry

- **4.1.1** Biological functions of biometals and role of metal ions in basic biological reactions
- **4.1.2** Dependence of biological growth on the concentration of essential and toxic metals

Diseases due to metal deficiency and its treatment (iron, zinc)

- **4.1.3** Metal ion toxicity
  - Toxic effects of metals (2 examples)
- **4.1.4** Detoxification of metal ion induced toxicity and clean up of toxic metals by plants
- **4.1.5** Thermodynamic and pharmacokinetic properties of chelating drugs (examples) Limitations of chelation therapy
- **4.1.6** Radioisotopes in medicine

#### 4.2 **Inorganic Pharmaceuticals**

- **4.2.1** Gastrointestinal agents viz. (i) antacids (aluminium hydroxide, milk of magnesia, sodium bicarbonate and (ii) cathartics (magnesium sulphate and sodium phosphate).
- **4.2.2** Topical agents viz. (i) protectives and adsorbents (talc, calamine), (ii) antimicrobial agents (potassium permanganate, tincture iodine, boric acid) and astringents (alum). Introduction to Platins.

# **CIA**: Assignment

#### REFERENCE BOOKS

- 1. James E. Huheey, Inorganic Chemistry-Principles of structure and reactivity, Harper & Row Publishers. London 1993
- 2. **D. F. Shriver and P.W. Atkins,** Inorganic Chemistry, 3<sup>rd</sup> edition., Oxford University Press.
- 3. F. A. Cotton, G. Wilkinson, C. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th ed., John Wiley, New York, 1999.

  4. **J. D. Lee,** Concise Inorganic Chemistry, 5<sup>th</sup> ed., Blackwell Science Ltd., 2005.

  5. **Gary Wulfsberg,** Inorganic Chemistry; Viva Books P A Ltd. New Delhi; 2010.

- 6. Gary L. Miessler and Donald A. Tarr, Inorganic Chemisty, 3<sup>rd</sup> edition, Pearson Education Inc. 2004.
- 7. **H.H. Jaffee and M. Orchin,** Symmetry in Chemistry, New Delhi, Wiley Eastern, 1965
- J. M. Hollas, Symmetry in Chemiostry, Chapman and Hall., NY, 1972
   F.A. Cotton, Chemical Application of Group Theory, 2<sup>nd</sup> edition, Wiley Eastern Ltd., New Delhi,
- 10. C.J. Ballhausen and H.B. Gray, Molecular Orbital Theory, McGraw-Hill, New York, 1965.
- 11. R. L. Dekock and H. B. Gray, Chemical Structure and Bonding, The Benjamin Cummins Publishing Company, 1980
- 12. A. R. West, Solid State Chemistry and its Applications, John Wiley & Sons, Singapore (2008)
- 13. Lesley Smart and Elaine Moore, Solid State Chemistry Introduction, 2<sup>nd</sup> Edition, Nelson Thornes Ltd., UK, 1996
- 14. Ulrich Muller, Inorganic structural Chemistry, 2<sup>nd</sup> edition, John Wiley and Sons. Chichester, 1993
- 15. R.N. Kutty and J. A. K. Tareen, Fundamentals of Crystal Chemistry, Universities Press (India) Ltd.
- 16. H. V. Keer, Principles of the Solid State, New Age International, 1993.
- 17. **D. K. Chakraborty**, Solid State Chemistry, New Age International Publishers, 1996.
- 18. N. N. Greenwood and A. Earnshaw, Chemistry of Elements, Pergamon, New York, 1984
- 19. H. Sisler, Chemistry in Non-aqueous Solvents, Reinhold Publ., New York, 1961
- 20. J. J. Lagowski, The Chemistry of Non-aqueous Solvents. Academic press, New York and London.
- 21. C. M. Day & J. Selbin, Theoretical Inorganic Chemistry, 2<sup>nd</sup> ed, Affiliated East West Press Pvt. Ltd., 1971

- 22. L.E. Orgel, An Introduction to Ligand Field Theory, Meuthen & Co. Ltd., London, 1960
- 23. **F. Basolo and R. G. Pearson,** Mechanism of Inorganic Reactions, 2<sup>nd</sup> ed, Wiley, New York, 1973
- 24. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, Wiley-Interscience, New York, 1988.
- 25. G. W. Parshall and S. D. Ittel, Homogenous Catalysis, 2<sup>nd</sup> edition, John Wiley & sons Inc., New York, 1992
- 26. Gary O. Spessard and Gary L. Miessler, Organometallic Chemistry, Prentice-Hall, (1997).
- 27. R. C. Mehrotra and A. Singh, Organometallic Chemistry A Unified Approach, 2<sup>nd</sup> ed. New Age International Pvt. Ltd. 2000
- 28. .B. Douglas, D. H. McDaniel and J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd edition, John Wiley & Sons, 1994
- 29. .F. A. Cotton and R. A. Walton, Multiple Bonds between Metal Atoms, 2<sup>nd</sup> edition, Clarandeen Press, Oxford, 1993
- 30. Sulabha K. Kulkarni, Nanotechnology-Principles and Practices, Capital Publishing Co., 2009
- 31. L. E. Smart and E. A. More Solid State Chemistry- An Introduction, 3<sup>rd</sup> edition, Taylor and Francis,
- 32. K. R. Mahadik and B. S. Kuchekar, Concise Inorganic Pharmaceutical Chemistry, Nirali Prakashan, Pune,
- 33. John H. Block, E. B. Roche, T. P. Soine and Charles O. Wilson, Inorganic Medicinal and Pharmaceutical Chemistry, Bombay, Varghese Pub house, 1986 Lea and Febiger, 1974.

  34. **G. S. Sodhi,** Fundamental Concepts of Environmental Chemistry, 3<sup>rd</sup> ed Narosa Publishing House,
- New Delhi, (2009)
- 35. M. L. Srivastava, Environmental chemistry, Shree Publishers & Distributors, New Delhi (2004)
- 36. **P.S. Sindhu**, Environmental Chemistry, New Age International (P) Ltd. New Delhi (2002)
- 37. B. Pani, Textbook of environmental chemistry, I. K International Publishing House Pvt. Ltd. New Delhi (2007)
- 38. G. M. Masters, Introduction to Environmental Engineering and Science, Prentice Hall of India Pvt. Ltd. New Delhi, 1995
- 39. Das, Asim, K. Inorganic Chemistry: Biological and Environmental Aspects

\*

SEMESTER 6 Course: No. S.CHE.6.03

# **SPECTROMETRIC IDENTIFICATION AND SYNTHETIC CHEMISTRY** 60 Lectures

UNIT I: Spectroscopy 15 L

- **1.1. Introduction:** Electromagnetic spectrum, units of wavelength and frequency.
- **1.2 UV-Visible Spectroscopy:** Basic theory, solvents, nature of UV-VIS spectrum, concept of chromophore, auxochrome, bathochromic shift, hypsochromic shift, hyperchromic effect and hypochromic effect. Chromophore-chromophore and chromophore-auxochrome interactions.
- **1.3 IR Spectroscopy:** Basic theory, nature of IR spectrum, selection rule, fingerprint region.
- **1.4 PMR Spectroscopy:** Basic theory of NMR, nature of PMR spectrum, chemical shift (δ unit), standard for PMR and solvents used. Factors affecting chemical shift: (a) inductive effect (b) anisotropic effect (with reference to C=C, C≡C, C=O and benzene ring). Spin-spin coupling and coupling constant. Proton exchange Application of deuterium exchange. Application of PMR in structure determination
- **1.5 Spectral characteristics** of the following classes of organic compounds, with respect to UV-VIS, IR, PMR (broad regions characteristic of different groups).:
  - (a) alkanes (b) alkenes and polyenes (c) alkynes (d) haloalkanes (e) alcohols (f) carbonyl compounds (g) ethers (h) carboxylic acids (i) esters (j) amines (k) amides (l) benzene and monosubstituted benzenes.
- **1.6 Mass Spectrometry:** Basic theory. Nature of mass spectrum. General rules of fragmentation. Importance of: molecular ion peak, isotopic peaks, base peak. Nitrogen rule. Illustrative fragmentation of alkanes and aliphatic carbonyl compounds (Mclafferty rearrangement not expected).
- **1.7 Problems on structure elucidation** of simple organic compounds using individual or a combination of spectra mentioned above. (index of hydrogen deficiency should be the first step in solving the problems).

#### **UNIT II: Name Reactions and Molecular Rearrangements**

15 L

- **2.1 Mechanism** of the following reactions with examples and synthetic applications:
  - (a) Claisen Condensation (b) Michael Reaction (c) Oppenauer Oxidation (d) Stobbe
  - Condensation (e) Wolff-Kishner Reduction.
- **2.2 Mechanism of rearrangements** with examples and stereochemistry wherever applicable:
  - (a) Pinacol-Pinacolone (b) Wolff (c) Beckmann (d) Hofmann (e) Baeyer-Villiger Oxidation.

**UNIT III : Synthetic Chemistry** 

15 L

# 3.1 Retro Synthetic Analysis

8 L

- **3.1.1 Introduction:** Definitions: (i) Disconnection (ii) Functional Group Interconversion (iii) Reagents (iv) Synthon (v) Synthetic equivalent (vi) Target Molecule.
- **3.1.2** Introduction to disconnections with respect to some simple molecules.
- **3.1.3** One Group Disconnections: Disconnection in molecules of alcohols, olefins, ketones.

# 3.2. Catalysts and Reagents

7 L

Study of the following catalysts and reagents with respect to functional group transformations and selectivity (no mechanism).

- **3.2.1. Catalysts:** Catalysts for hydrogenation: Raney Ni, Pt and PtO<sub>2</sub>: C=C, CN, NO<sub>2</sub>, aromatic ring; Pd/C: C=C, COCl □ CHO (Rosenmund); Lindlar catalyst: alkynes; Wilkinson's catalyst for stereoselective reduction of olefins.
- **3.2.2 Reagents**: (a) LiAlH<sub>4</sub> and Red-Al: reduction of CO, COOR, CN, NO<sub>2</sub>.
  - (b) NaBH<sub>4</sub>: reduction of CO. (c) Diborane: olefins to alcohols through hydroboration, reduction of COOH. (d) SeO<sub>2</sub>: hydroxylation of allylic and benzylic positions, oxidation of CH<sub>2</sub> alpha to CO to CO. (e) *m*CPBA and H<sub>2</sub>O<sub>2</sub>/NaOH for epoxidation of enones. (f) NBS: allylic and benzylic bromination and bromination of position alpha to CO.
  - **3.2.3 Organolithium compounds:** Preparation using alkyl/aryl halides. Reactions with compounds containing acidic hydrogen, alkyl halides, carbonyl compounds, cyanides and CO<sub>2</sub>. **Lithium dialkyl cuprates:** Preparation and reactions with **aliphatic/ aromatic/ vinylic**

UNIT IV 15 L

4.1 Polymers

halides.

15 L

- **4.1.1 Introduction:** General idea of monomers, polymers, and polymerization. natural and synthetic polymers. Homopolymers and copolymers. Classification of polymers. Copolymers alternating, block, random and graft.
- **4.1.2 Mechanism** of free radical addition polymerisation.
- **4.1.3** Elastomers: Natural and synthetic rubbers. Diene polymerization: 1,2-and 1,4-addition (*cis* and *trans*) polymerization of isoprene. 1,3-Butadiene- styrene copolymer.
- **4.1.4 Stereochemistry of polymers:** Tacticity. Role of Ziegler–Natta catalyst (coordination polymerization) in directing the tacticity in polypropylene (no mechanism).
- 4.1.5 Preparation and uses of polymers:
- (a) Addition polymers: (i) polyethylene (ii) polypropylene (iii) PVC
  - (iv) polystyrene (v) polyacrylonitrile (vi) polyvinylalcohol (vii) teflon. (b)
- Condensation polymers: (i) polyesters (ii) polyamides (iii) polyurethans
  - (iv) phenol-formaldehyde resin (v) epoxy resin (vi) polycarbonates.
- **4.1.6 Recyclable polymers:** Biodegradable polymers and their uses. Biomedical uses of polymers.
- **4.1.7** Additives to polymers: Plasticizers, stabilizers and filler

(Students are expected to identify monomers in a given polymer and draw the structure of a polymer from a given set of monomers).

**CIA II:** Problem solving based on Spectroscopy and Retrosynthesis.

# **Reference Books:**

- Francis A Carey, Organic Chemistry, Pearson Education, 7<sup>th</sup> Edition, Tata McGraw Hill, (1)
- **R.T. Morrison and R.N. Boyd,** Organic Chemistry, 6<sup>th</sup> Edition, Pearson Education.2008 (2)
- **G. Marc Loudon**, Fundamentals of Organic Chemistry, 4<sup>th</sup> Edition, Oxford University (3) Press, 2006.
- **L.G. Wade Jr. and M.S. Singh,** Organic Chemistry, 6<sup>th</sup> Edition, Pearson Education, New (4) Delhi, 2008.
- (5)
- **Paula Y. Bruice,** Organic Chemistry, 3<sup>rd</sup> ed, Pearson Education, 2007. **J.G. Smith,** Organic Chemistry, 2<sup>nd</sup> Edition, Special Indian Edition, Tata McGraw Hill, (6) New Delhi, 2008.
- **S.H. Pine,** Organic Chemistry, 5<sup>th</sup> ed, McGraw Hill Kogakusha Ltd.2007 (7)
- **J. McMurry**, Organic Chemistry, 5<sup>th</sup> Edition, Asian Books Pvt. Ltd., New Delhi, 2006. (8)
- Peter Sykes, A guide to mechanism in Organic Chemistry, 6<sup>th</sup> Edition, Pearson (9) Education, New Delhi.
- V.K. Ahluwalia and R.K. Parashar, Organic Reaction Mechanism, 4<sup>th</sup> ed., Narosa (10)Publications.
- **P.S. Kalsi,** Stereochemistry, conformation and mechanism, 7<sup>th</sup> ed, New Age International Ltd., 2008.
- (12) **E. L. Eliel,** Stereochemistry of Carbon compounds, Tata McGrawHill, New Delhi.
- (13) V.K. Ahluwalia, Textbook of Organic Chemistry, (Vol 1 3), Ane Books Pvt Ltd 2010
- (14) **P.S. Kalsi,** Stereochemistry through solved problems, Wiley Eastern, 1994
- (15) **P.S. Kalsi,** Spectroscopy of Organic compounds, New Age International Ltd, 1995
- **Jagmohan**, Organic Spectroscopy- Principles and Applications- 2<sup>nd</sup> ed., Narosa (16)Publication.2008
- (17) **W. Kemp,** Organic Spectroscopy, 3<sup>rd</sup> Edition, Palgrave, Indian Edition, 2005.
- Williams and Fleming, Spectroscopic methods in Organic Chemistry, 5<sup>th</sup> ed, McGraw (18)Hill 1995
- **B.G. Devis and A.J. Fairbanks,** Carbohydrate Chemistry, Oxford University Press, New Delhi, Indian Edition, 2005.
- D. Walton and P. Lorimer, Polymers, Oxford University Press, New Delhi, Indian Edition, 2005.
- (21) V.K. Ahluwalia, Terpenoids, Ane Books Pvt. Ltd., New Delhi, 2009.
- (22) V.K. Ahluwalia and A. Mishra, Polymer Science, Ane Books Pvt. Ltd., New Delhi, 2009.
- (23) V.K. Ahluwalia, An introduction to Green Chemistry, Vishal Publishing Co.
- (24) **K.S. Tewari, N.K. Vishnoi,** Organic Chemistry, Vikas Publications.

- (25) N.K. Vishoi, Advanced Practical Organic Chemistry, 2<sup>nd</sup> Edition, Vikas Publications.
   (26) I.L.Finar, Organic Chemistry, 6<sup>th</sup> ed Volume 2 Stereochemistry and the Chemistry of Natural Products, Fifth Edition, Pearson.
- Satyanarayan Biochemistry (27)
- (28) Stuart Warren, Designing Organic Syntheses, Wiley India Pvt. Ltd., 2009.

\*

SEMESTER 6 Course: No. S.CHE.6.04

#### INSTRUMENTAL METHODS OF ANALYSIS

60 Lectures

## **Learning Objectives:**

- 1. To expose students to instrumental techniques involving sophisticated instruments that are commonly used in industry
- 2. To understand the principles, theory, instrumentation and applications of instrumental methods
- 3. To understand the need for validation of analytical methods
- 4. To familiarize students with concept of quality and good laboratory practices

## **UNIT I: Optical Methods:**

15 L

- **1.1. UV-Visible spectrophotometry:** Instrumentation of single and double beam spectrophotometer. Quantitative analysis: calibration curve method.
- **1.2. Atomic spectroscopy:** Absorption and emission spectra, energy level diagrams, processes involved in atomization. Flame photometry: flame atomizer, types of burners, monochromators and detectors. Atomic absorption spectroscopy: flame and electrothermal atomizer, hollow cathode lamp, construction and working of instruments. Quantitative applications of atomic absorption spectroscopy and flame photometry. Calibration curve method, standard addition method and internal standard method.
- **1.3**. **Turbidimetry and Nephelometry:** scattering of light, effect of concentration, particle size and wavelength on light scattering, instrumentation and applications.

## **UNIT II: Electroanalytical Methods**

15 L

- **2.1. Potentiometric Titrations:** Principles, titration curves and location of equivalence point in acid-base and redox titrations, applications.
- **2.2. D.C. Polarography:** Polarizable and nonpolarizable electrodes, basic principles of polarography, polarographic cell, residual current, diffusion current, limiting current, dropping mercury electrode, supporting electrolyte, half wave potential. Derivation of the polarographic wave equation for a reversible reaction, Ilkovic equation, oxygen interference and its removal, polarographic maxima and maxima suppressors, qualitative and quantitative analysis, calibration curve and standard addition method, applications. {Numerical problems expected}
- **2.3. Amperometric Titrations:** Basic principles, rotating platinum electrode, nature of the titration curves, applications, advantages and limitations.

UNIT III 15 L

# **3.1.** Chromatographic Methods:

12 L

- **3.1.1.Gas chromatography:** gas liquid chromatography, basic principles, retention time, retention volume, resolution, peak width, theoretical plates, HETP, instrumentation, columns, detectors, applications.
- **3.1.2.High performance liquid chromatography**: instrumentation, types of stationary phases, types of elution, U.V. and R.I. detector and applications.
- **3.1.3. HPTLC:** instrumentation, applications

## 3.2. Introduction to Radio-analytical Methods

3 L

**3.2.1. Neutron Activation Analysis:** theory, technique and applications

UNIT IV 15 L

#### 4.1 Thermal methods:

4 L

**4.1.1 Thermogravimetric Analysis:** basic principles, instrumentation, factors affecting the TG curve, applications.

# 4.2. Analytical method validation and Total Quality Management:

11 L

- **4.2.1.** Need for validation of an analytical method
- **4.2.2** Parameters of method validation.
- **4.2.3.** Total quality management: concept of quality, Quality Control, Quality Assurance, Total Quality Management,
- **4.2.4** ISO series, Good Laboratory Practices.

CIA: Instrumentation, including Schematic diagrams of instruments

#### **Reference Books:**

- 1 **D. A. Skoog, D.M.West, F.J.Holler** Fundamantals of Analytical Chemistry, 8<sup>th</sup> ed. Philadelphia, Saunders college Publishing, 1996
- 2 **D. A. Skoog, F.J.Holler, T.A.Nieman,** Principles of Instrumental Analysis, 6<sup>th</sup> ed. Philadelphia, Saunders college Publishing, 1996
- 3 **G.D.Christian,** Analytical Chemistry, 6<sup>th</sup> ed. John Wiley &Sons, Singapore, 2004.
- 4 **J.G.Dick,** Analytical Chemistry, International Student's Edition, McGraw Hill, Kogakusha Limited, New Delhi, 1973.
- 5 **R.A.Dey & D.L.Underwood,** Quantitative Analysis, 6<sup>th</sup> ed. Prentice Hall Of India Pvt. Ltd. New Delhi, 1993.
- 6 **M.Valcarcel,** Principles Of Analytical Chemistry, Springer International Edition, Berlin, 2000
- 7 E..Prichard, & V. Barwick, Quality Assurance in Analytical Chemistry, Wiley.
- 8 **S. M. Khopkar,** Basic Concepts of Analytical Chemistry, 3<sup>rd</sup> ed,New Age International Publishers, 2008

- **S. M. Khopkar,** Analytical Chemistry Problems and Solutions, New Age International Publishers, 2002
- **A I Vogel,** Textbook of Quantitative Chemical Analysis, 6<sup>th</sup> ed, Pearson Education, 2002
- **Kolthoff and Elving,** Treatise on Analytical Chemistry, Part I Vol 1, Interscience Encyclopedia 1959
- **J M Miller**, Separation methods in Chemical Analysis, John Wiley, 1975
- **J A Dean,** Chemical Separation Methods, 1969
- **R.D. Braun,** Introduction to Instrumental methods of Analysis, McGraw Hill, 1987
- **G R Chatwal and S K Anand**: Instrumental methods of Chemical Analysis, 5<sup>th</sup> ed, Himalaya Publishing House, 2002
- **H H Willard, L L Merritt and J A Dean**; Instrumental methods of Analysis, 7<sup>th</sup> ed CBS Publishers, 1986
- **A K Srivastava, P C Jain,** Chemical Analysis, an Instrumental Approach 3<sup>rd</sup> ed , S Chand 1997
- **G W Ewing**, Instrumental methods of chemical analysis, 5<sup>th</sup> ed, McGraw Hill, 1976
- 19 Ed Newman, N T Crosby, J A Day, Quality in the Analytical laboratory, Wiley, 2008
- 20 Value engineering and quality assurance, IGNOU School of Management studies, 1993

\*

Semester 6 Course No: S.CHE.PR.6

# **Course 6.01: Physical Chemistry**

# **Non Instrumental Experiments**

# **CHEMICAL KINETICS**

- 1. To determine the energy of activation of acid catalyzed hydrolysis of methyl acetate.
- 2. To study the effect of ionic strength (KCl) on the reaction between K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> and KI.
- 3. To study the Saponification of ethyl acetate with sodium hydroxide at equal concentrations of ester and alkali.

# **PARTITION COEFFICIENT**

- 4. To determine the partition co-efficient of  $I_2$  between  $CCl_4$  and  $H_2O$ .
- 5. To determine the equilibrium constant for the reaction  $KI + I_2 = KI_3$  by partition method.

# ADSORPTION EXPERIMENT

6. To study the adsorption of acetic acid / oxalic acid on charcoal.

#### PHASE RULE

7. To determine the phase diagram for the system water, chloroform, acetic acid at room temperature.

# SOLUBILITY MEASUREMENT

**8.** To determine the solubility product of calcium hydroxide at room temperature.

#### **VISCOSITY**

- **9.** To determine the molecular weight of polyvinyl alcohol by viscosity measurements.
- 10. To determine the size (radius) of a glycerol molecule by viscosity.

# **Course 6.02 : Inorganic Chemistry**

# 1. Gravimetric Analysis

- (i) Estimation of Barium as Barium Chromate in the presence of Iron.
- (ii) Estimation of Nickel as Nickel dimethyl glyoxime in the presence of Copper.

# 2. Inorganic Preparations

- (i) 8-(Hydroxyquinolinato) magnesium (II).
- (ii) Nickel dimethyl glyoxime.
- (iii) Copper chloride dimethyl sulfoxide.

# 3. Titrimetric analysis

- (i) Estimation of Cobalt by EDTA method using Xylenol Orange.
- (ii) Estimation of Aluminium using EDTA.

## **Course 6.03: Organic Chemistry**

# [A] Organic Separation:

**Separation of a binary mixture:** Type of mixture, Separation and identification (**microscale**) of both components through systematic scheme of identification.

Types: Solid + Solid, Volatile Liquid + Solid, Volatile Liquid + Nonvolatile Liquid (No carbohydrates to be given).

Mass of solid: ~ 3-4g, Liquid: Volatile ~ 6-8mL, Nonvolatile ~ 4-6 mL

# [B] Preparation of Organic compounds:

Preparation of Organic compound as per the procedure given. Measuring the mass of crude, purification of the separated product by crystallization and recording of the m.p. Quantity of reactant to be given 1g.

- 1) Benzaldehyde/p-nitrobenzaldehyde  $\square$  Acid (oxidation).
- 2) Acetanilide 

  p-bromoacetanilide
- 3) p-Bromoacetanilide to p-bromoaniline
- 4) m-Dinitrobenzene □ m-nitroaniline.

**Note:** A minimum 6 mixtures and 3 preparations should be covered in each semester

# **Course 6.04: Analytical Chemistry**

# **Instrumental Experiments**

- 1. Determination of amount of Fe (III) present in the given solution by EDTA titration Colorimetrically.
- 2. Determination of the amount of fluoride in the given solution colorimetrically.
- 3. Determination of potassium content of a commercial salt sample by flame photometry using Calibration Curve Method.
- 4. Estimation of sodium in given solution by flame photometry using Standard Addition Method.
- 5. Estimation of aspirin / Vitamin C content of a tablet by pH metry.
- 6. Estimation of acetic acid in vinegar using potentiometric titration.
- 7. Determination of the amount of iron present in the given vitamin tablet colorimetrically.
- 8. Determination of HCl and H<sub>2</sub>SO<sub>4</sub> in a mixture by titration with NaOH and BaCl<sub>2</sub>.
- 9. Determination of Glucose by Folin-Wu method colorimetrically.
- 10. Nephelometric determination of sulphate.

## **References:**

- 1. Panday, O.P., D. N. Bajpai and S. Giri, *Practical Chemistry*, Delhi: S. Chand, 2008.
- 2. V.D.Athawale and P. Mathur, Experimental Physical Chemistry: New Age International. 2008

# **PRACTICAL**

# **❖ CIA AND END SEMESTER PRACTICAL EXAMINATION**

**Course 6.01**: Physical Chemistry – Non –Instrumental experiment

**Course 6.02:** Inorganic Chemistry – Gravimetric analysis

**Course 6.03:** Organic Chemistry – Separation and Identification of liquid-liquid and liquid-

Solid mixture.

Preparation of Organic compounds

**Course 6.04:** Analytical Chemistry – Instrumental Experiment.

**Journal**: 5 marks per course.

**CIA:** 15 marks per course.

**Duration**: 4 periods to be conducted during regular practicals by the Faculty-in- charge.

One or more practical skills will be tested in the CIA.

**End Semester Examination**: 30 marks per course. This includes a 5 mark viva-voce based on the theory behind all the experiments conducted per course.

There will be an External Examiner and an Internal Examiner responsible for two courses each.

**Duration**: 3½ hrs per course.

**Batch size**: Max 20 students per batch for courses 2 and 3 and 10 students per batch for courses 1 and 4 (involving instruments).

# **SEMESTER 6**

# DRUGS AND COLOR CHEMISTRY FOUR CREDIT COURSE

# **Learning Objectives:**

- 1) To familiarize students with the mode of action of drugs.
- 2) To understand the uses and the side effects of certain drugs for various diseases.
- 3) To study the synthesis of different drugs
- **4)** To study the nomenclature and characteristics of dyes.
- 5) To study the concept of colour and its relation to chemical structure.
- **6**) To familiarize the students with the types of fibres, application of dyes and how the dyes are attached to them.
- 7) To familiarize the students with the syntheses of some representative dyes.
- 8) To create an awareness of the current concern about the toxicity of dyes and their effect on ecology.

UNIT I 15 L

# 1.1 General Introduction to drugs.

7 L

Course No: S.CHE.6.AC

60 L

- **1.1.1:** Definition of drug, requirement of an ideal drug, classification of drugs (based on Therapeutic action )
- **1.1.2:** Nomenclature of drugs, generic name, brand name, systematic name.
- **1.1.3:** Definition of the following medicinal terms: Pharmacon, Pharmacophore, Prodrug, Half-life efficiency, LD<sub>50</sub>, ED<sub>50</sub>, Therapeutic index.
- **1.1.4:** Brief idea of the following terms: receptors, drug-receptor interaction, drug potency,

Bioavailability, drug toxicity, drug addiction, spurious drugs, misbranded drugs,

Adulterated drugs, Pharmacopoeia.

## 1.2 Routes of drug administration and dosage forms:

3 L

- **1.2.1:** Oral and parenteral routes with advantages and disadvantages.
- **1.2.2:** Formulations, different dosage forms (emphasis on sustained release formulations.)

6 <sup>th</sup>	Semester Syllabus for Core Component Course in Chemistry, St. Xavier's College -
	Autonomous, Mumbai

# 1.3 Synthesis of following drugs.

5 L

Paracetamol, Aceclofenac, Salbutamol, Ciprofloxacin, Metronidazole, Mebendazole, Ethambutol, 5-Fluorouracil, Atenolol, Dapsone and Trimethadione.

UNIT II 15 L

# 2.1 Pharmacodynamic agents

9 L

A brief introduction of the pharmacodynamic agents and study of their chemical class, Chemical structure, therapeutic uses and side effects.

- 2.1.1: Analgesics (Narcotics and non-narcotics) and Antipyretics: Classification of analgesics: narcotics and non narcotics. Morphine (phenanthrene alkaloids), Tramadol, Aspirin(salicylates), Paracetamol (p-amino phenol)
- 2.1.2: Anti-inflammatory drugs: Mechanism of inflammation and various inflammatory conditions: Prednisolone, Betamethasone (steroids), Aceclophenac (aryl acetic acid), Mefenamic acid (N-aryl anthranilic acid.)
- 2.1.3: Drugs for respiratory system: General idea of Expectorant, Mucolyte,
  Bronchodialators, Decongestants and Antitussives. Bromhexine (phenyl methyl amines),
  Salbutamol, Pseudo-ephedrine (phenyl ethyl amines), Oxymetazoline (imidazolines),
  Codeine phosphate (opiates)
- **2.1.4: Drug** metabolism: Introduction, absorption, distribution, bio-transformation, excretion, different types of chemical transformation of drug with specific examples .

# 2.2 Chemotherapeutic agents

6

A brief introduction of the chemotherapeutic agents and study of their chemical class, chemical structure, therapeutic uses and side effects.

- **2.2.1:** Antibiotics: Definition, characteristics and properties: Amoxicillin, Cloxicillin (β-lactum antibiotic), Cephalexin (cephalosporins), Doxycycline (tetracyclines), Ciprofloxacin (quinolone)
- **2.2.2:** Antitubercular and antileprotic drugs: Study of tuberculosis types, symptoms, and diagnosis of tuberculosis.

Types of leprosy: General idea of antibiotics used in their treatment: PAS (aminosalicylates), Isoniazid (hydrazides), Pyrazinamide (pyrazine), (+) Ethambutol (aliphatic diamines), Ethionamide (thioamides), Dapsone(sulfonamides), Clofazimine(phenazines). Combination therapy to be discussed.:

- i)Rifampicin +Ethambutol +Pyrazinamide.
- ii)Rifampicin +Isoniazide + Pyrazinamide.
- iii)Rifampicin + Clofazimine + Ethionamide.

Unit III:

# 3.1 : Introduction to dyestuff chemistry

3 L

- **3.1.1** : Definition of dyes, properties (colour and fastness).
- **3.1.2** : Important milestones in the development of synthetic dyes.
- **3.1.3** : Nomenclature of commercial dyes with at least one example.

Suffixes – G, O, R, B, 6B, L, S; colour index and colour index number.

# 3.2 : Classification of dyes based on constitution

3 L

(Examples as mentioned below with structures)

- I : Nitro dyes Naphthol Yellow S
- II : Nitroso dyes Gambine Y
- III: Azo dyes
  - a) Monoazo dyes Orange IV
  - b) Disazo dyes Congo Red
  - c) Trisazo dyes Direct Deep Black
- IV: Diphenylmethane dyes Auramine O

- V: Triphenylmethane dyes
  - a) Diamines Malachite Green
  - b) Triamines Crystal Violet
  - c) Phenols Phenolphthalein

VI: Heterocyclic dyes –

- a) Xanthenes Eosine
- b) Azines Safranine-T
- c) Thiazines Methylene Blue

VII: Anthraquinone dyes- Alizarin, Alizarin Cyanine Green G, Indanthrone

VIII: Indigoide dyes- Indigo

IX: Phthalocyanines-Monastral Fast Blue BS

# 3.3 : Classification of dyes based on application

6 L

Definition, fastness properties and applicability on substrates, examples with structures.

- a) Acid dyes Orange II, Alizarin Cyanine Green G.
- b) Basic dyes Crystal Violet, Bismark Brown.
- c) Direct Cotton Dyes Chrysophenine G.
- d) Azoic dyes Diazo components: Fast Red B Base, Fast Blue B Base; Coupling components: Naphtol AS, Naphtol AS-G.
- e) Mordant dyes Eriochrome Black T, Alizarin.
- f) Vat dyes Indigo, Indanthrene.
- g) Disperse dyes-Celliton Scarlet B, Disperse Yellow 6G
- h) Fluorescent dyes-Rhodamine B

# 3.4 : Colour and chemical constitution of dyes

3 L

3.4.1 Absorption of visible light, colour of wavelength absorbed and complementary colour, chromogen, chromophore, auxochrome, bathochromic and hypsochromic shifts.

3.4.2	:	Rela	ation of colour to resonance in the following classes of dyes: Azo,			
		Trip	henylmethane, Anthraquinone.			
Unit I	V	:		15L		
4.1	:	Org	anic Pigments	2 L		
		orga exai	eral idea, difference between dyes and pigments. Important characteristics of inic pigments, toners and lakes. Classification of organic pigments with suitable imples, i.e. ionic pigments (lakes of acid and basic dyes), nonionic pigments (azgoids, anthraquinone), uses of pigments.			
4.2	:	Syn	thesis of specific dyes and their uses	7 L		
		i)	Orange IV from sulphanilic acid			
		ii)	Bismark Brown from m-phenylenediamine			
		iii)	Malachite Green by using benzaldehyde and N,N-dimethylaniline			
		iv)	Methylene Blue by using 4-amino-N,N dimethylaniline and N,N dimethylanil	ine		
		v)	Congo Red from nitrobenzene			
		vi)	Eriochrome Black T from $\beta$ – naphthol			
		vii)	Alizarin from anthraquinone			
		viii)	Indigo from aniline			
		ix)	Indanthrene from anthraquinone			
		x)	Disperse Yellow 6G from benzanthrone			
4.3	:	Тур	es of fibres and classes of dyes applicable to it	2 L		
4.3.1	1 : Introduction to the following types of fibres with structures and classes of dye					
		appl	icable to these fibres: Cotton, wool, silk, polyester.			
4.4	:	For	ces binding dyes to the fibres: Ionic forces, hydrogen bonds,	2 L		
		Van	der Waal's forces, covalent linkages.			
4.5	:	Bas	ic operations involved in a dyeing process	1 L		

Preparation of fibre for dyeing, preparation of the dye bath, application of the dye

6<sup>th</sup> Semester Syllabus for Core Component Course in Chemistry, St. Xavier's College – Autonomous, Mumbai

And finishing

# 4.6 : Ecology and toxicity of dyes

**1L** 

Brief idea of environmental pollution and health effects due to dyes.

# **REFERENCES**

- 1) Pharmacology and pharmaceutics Vol.I and II, Satoskar
- 2) Textbook of organic, medicinal, and pharmaceutical chemistry, Wilson and Gisvold
- 3) Textbook of medicinal chemistry, William O. Foye and David A. William
- 4) Medicinal chemistry, G. R. Chatwal
- 5) Chemistry of synthetic dyes, Vol. I to VI, K. Venkataraman
- 6) Chemistry of synthetic dyes and pigments, H. A. Lubs
- 7) Colour Chemistry, H. Zollinger
- 8) Colour Chemistry, R. L. M. Allen
- 9) Unit process, Groggins
- 10) Synthetic dyes, M. S. Yadav
- 11) Physical Chemistry of dyeing, Thomas Vickerstaff
- 12) Chemistry of dyes and principles of dyeing, V. A. Shenai
- 13) Practical Organic Chemistry, A. I. Vogel

CIA I : Short answer questions 20 MARKS

CIA II: Questions on syntheses of drugs and dyes 20 MARKS

# **Template of Question Paper**

# DRUGS AND COLOR CHEMISTRY

# **OBJECTIVES**

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL MARKS
I	6	6	3	15
II	6	6	3	15
III	6	6	3	15
IV	6	6	3	15
TOTAL MARKS PER OBJECTIVES	24	24	12	60
% WEIGHTAGE	40	40	20	100

**End Semester Paper Pattern:** 

Total marks: 60 Maximum time: 2 hours

Total no. of questions: 4 [all compulsory] of 15 marks each

1 question per unit:

Questions set out of 22 marks [50 % internal choice]

Sub questions will not exceed 5 marks

**COURSE: S.CHE.6.AC.01** 

# SYLLABUS UNDER AUTONOMY CHEMISTRY

PRACTICAL COURSE IN T.Y.B.Sc. COURSE: S.CHE.6.AC.01.PR

#### I. PREPARATIONS

- 1. Aspirin from Salicylic acid.
- 2. p-Nitroacetanilide from Acetanilide.
- **3.** p-Nitroaniline from p-Nitroacetanilide.
- 4. m-Dinitrobenzene from Nitrobenzene
- 5. Fluorescein from Phthalic Anhydride
- **6.** Anthraquinone from Anthracene

# II. ESTIMATIONS

- 1. Estimation of Iodine in Tincture Iodine
- 2. Estimation of Ibuprofen
- 3. Estimation of Methyl Orange/Eriochrome Black T/Congo Red by colorimetry

CIA: ESTIMATION OF DRUG/DYE

JOURNAL

5 Marks

END SEMESTER PRACTICAL EXAMINATION

30 MARKS

## PREPARATION OF DRUG/DYE

The practical exam will be conducted for 1 session of 3 hours duration.

**BATCH SIZE FOR:** 

REGULAR PRACTICALS 20 STUDENTS PER IN-CHARGE

EXAMINATIONS MAXIMUM 20 STUDENTS PER BATCH

\*

\*