

# St. Xavier's College (Autonomous), Ahmedabad-09

## M Sc Chemistry

### Overview

Note:- Semester -I and Semester-II syllabus is common for all specializations to be selected by the students for final year i.e. Inorganic, Organic, Physical and Analytical. At present St. Xavier's College offers only Organic Chemistry as a specialization in the final year of M Sc Chemistry.

### M Sc Semester I

**CORE Paper: Inorganic Chemistry (Theory)**

**Course Code: PCH 1801**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

### Course Overview & Course Objectives

The main objective of the course will be to enhance the understanding and knowledge of Inorganic Chemistry, for students studying, any branch of chemistry.

By the end of the paper, a student will be able to:

- Understand the important aspects of Quantum theory and Atomic Structure
- Know and study the Symmetry and Group Theory
- Understand the important aspects of Magneto chemistry
- Know and study Bio-inorganic Chemistry

Thus, the knowledge from the course can help in the following:

- Finally, all students, of all branches whether organic or inorganic will be able to incorporate this knowledge, in their pursuit of research in their different fields.

### Course Content

**Unit-1: Quantum theory and Atomic Structure**

**(15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Quantum theory and Atomic Structure]

Postulates of quantum mechanics, setting up of different observables, commutation relations, step-up and step-down operators. Simple harmonic oscillator. Angular momentum of inner quantum number  $j$ .

Approximation methods: Variation method and application to H atom. Perturbation theory (first order and non-degenerate), application to the Helium atom.

**Unit-2: Symmetry and Group Theory****(15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Symmetry and Group Theory]

Representation of groups –some properties of matrices & vectors, representation of groups, the Great orthogonality theorem and its consequences, character table, wave functions as basis for irreducible representations, direct product, identifying non- zero matrix elements.

**Unit-3: Magnetochemistry****(15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Magneto chemistry]

Magnetic susceptibility and basic derivation of diamagnetic susceptibility, pascal constant and its utility, Curie law and Curie-Weiss law, antiferromagnetism and ferromagnetism. Types of antiferromagnetism, antiferromagnetic exchange pathway: Direct –metal- metal interaction and Indirect-atom exchange i.e. super exchange mechanism.

**Unit-4: Bio-inorganic Chemistry****(15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Bio-inorganic Chemistry]

Metalloporphyrins (enzymes) definition, hemoglobin and myoglobin, cytochrome, vitamin B<sub>12</sub> (cyanocobalamin), zinc metallo enzymes, nitrogen fixation, essential and trace elements in biological system, biochemistry of non metals K, Na pump (action of bath ions), toxic metals and their toxicity.

Co-ordination compounds in medicine

Chelation therapy, gold compounds and rheumatoid arthritis, anticancer drugs –platinum complexes, gold complexes, metallocenesetc, antimicrobial agents, metal complexes as radio diagnostic agents, magnetic resonance imaging.

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

**Reference Books: PCH 1801: Inorganic Chemistry (Theory)**

1. Introduction to Quantum Chemistry, A. K. Chandra, Tata MacGraw Hill
2. Quantum Chemistry, Ira N. Levine, Prentice Hall
3. Quantum Chemistry by R. K. Prasad, New Age International Publishers (1985)
4. Elementary Quantum Chemistry by D. L. Pilar, McGraw Hill Book Co, New York (1968)
5. D. A. McQuarrie Quantum Chemistry, OUP 1983

6. M. W. Hanna, Quantum Mechanics in Chemistry, The Benjamin Pub.
7. Molecular Quantum Mechanics, Third Edition, P. W. Atkins and R.S. Friedman
8. Group theory and symmetry in chemistry, L. H. Hall(McGraw Hill)
9. F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern 2nd Edn.1992
10. V. Ramkrishnan& M. S. Gopinadhan, Group theory in Chemistry Vishal Pub.1996.
11. Inorganic Chemistry, Third Edition, Alan G. Sharpe
12. Theoretical Inorganic Chemistry, M. C. Day, J. Shellin
13. Chemistry, Fifth Edition, John E. McMurry, Robert C. Fay
14. Hermann Dugas, Bioorganic Chemistry, A Chemical Approach to Enzyme Action, Springer International Edition
15. An Introduction to Theoretical Chemistry, Jack Simons, Cambridge
16. Progress in inorganic Chemistry, Vols 18 and 38 ed. J. J. Lippard, Wiley
17. Inorganic Reaction Mechanisms, M. L. Tobe, Nelson Pub
18. Inorganic Chemistry, K. F. Purcell and J. C. Kotz.
19. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Bers
20. Bioinorganic Chemistry, I. Bertini, H. B. Gray and S. J. Lippard
21. Principals of Bioorganic Chemistry, S. J. Lippard and J. M. Berg, University Science Books.
22. Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, University Science Books.
23. Inorganic Biochemistry vols I and II ed. G. L. Eichhorn, Elsevier
24. Introduction to Magnetochemistry, Alan Earnshaw, 1968
25. Elements of Magnetochemistry, Dutta and Syamal, 1993

### Semester I

**Paper: PCH 1802: Organic Chemistry (Theory)**

**CORE Paper: Organic Chemistry (Theory)**

**Course Code: PCH 1802**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

### Course Overview & Course Objectives

The main objective of the course will be to enhance the understanding and knowledge of organic chemistry

By the end of the paper, a student will be able to :

- a. Understand the details of Elimination Reaction and Nucleophilic Substitution Reaction
- b. The chemistry of various types of Molecular rearrangement reactions.
- c. Understand the important aspects of Reactive intermediates and Aromaticity
- d. Understand the details of various aspects of Stereo Chemistry.

Thus, the knowledge from the course can help in the following:

This content can help students to increase their conceptual base and understanding in these topics which will be needed by students in their pursuit of research in other allied branches of chemistry.

## Course Content

### Unit-1:

(15L) [14Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Elimination Reaction and Nucleophilic Substitution Reaction]

#### 1. Elimination Reaction

The E1, E2 and E1CB reaction mechanism. reactivity- effects of substrate structures, attacking base, leaving group and medium. Regiochemistry of E1 and E2 elimination reactions. Stereochemistry of E2eliminations in cycloalkane and related systems. Mechanism and orientation in Pyrolytic eliminations in (1) Acyclic systems (ii) Alicyclic systems (iii) Cope eliminations. Thermal decomposition without rearrangement. - The chugaev reaction.

#### 2. Nucleophilic Substitution Reaction

Mixed  $S_N^1$ ,  $S_N^2$  and SET mechanism. Nucleophilic substitution at (i) Allylic carbon (Allylic rearrangements) (ii) An Aliphatic trigonal carbon (the tetrahedral mechanism) and at (iii) A Vinyl carbon. Participation of Neighboring groups in Nucleophilic substitution by (a) Carboxylate anion (b) Halogen atoms (c) Hydroxyl groups (d) Acetoxy group (e) Phenyl group (f) RS group (g) Participation by  $\pi$ -bond.

### Unit-2: Molecular rearrangements

(15L) [14Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Molecular rearrangements]

Introduction: Definition and classification.

#### 1. Rearrangements Induced by Cationic or Electron Deficient Sites

Molecular rearrangements involving electron deficient carbon:

- (i) Wagner- Meerwein
- (ii) Pinacol- Pinacolone rearrangement
- (iii) Tiffeneau-Demjanov Rearrangement

Rearrangements to Electron Deficient Heteroatoms

A) Electron deficient Nitrogen:

- (i) Lossen rearrangement
- (ii) Curtius rearrangement
- (iii) Schmidt rearrangement

B) Electron deficient Oxygen:

- (i) Baeyer-Villager Rearrangement

## 2. Rearrangements Induced by Bases or Electron Rich Sites

- (i) The Favorskii Rearrangement
- (ii) Wittig and Stevens Rearrangement
- (iii) Benzylic acid rearrangement
- (iv) The Sommelet-Hauser rearrangement

### Unit-3:

(15L) [14Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to reactive intermediates and aromaticity]

#### 1. Reactive intermediates

Carbocations (classical and non classical), Carbanion, Carbenes, Free radicals and Nitrenes: their stability, structure, generation and fate.

#### 2. Aromaticity

Aromaticity, aromatic character, Frost circle diagram for cyclobutadiene, benzene and others. Resonance and chemical stabilization-aromatic character based on NMR criteria, Huckels molecular orbital (HMO) method, MO of simple organic systems such as ethene, allyl and butadiene. Aromaticity in benzenoid and non-benzenoid compounds and charged rings, annulenes, fulvenes, azulenes, antiaromaticity and homoaromaticity.

### Unit-4: Stereo Chemistry

(15L) [14Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Stereo Chemistry]

Planar and helical Chirality: Configurational nomenclature: Planar chiral ANSA compounds and trans- cyclooctene. Helical chiral compounds. Enantioselective Synthesis – Epoxidation of allyl alcohols (Sharplessepoxydation), Enantioselectivity through Hydroboration-Oxidation, Enantioselectivity through use of Phase transfer catalysts, Reduction of ketones with chiral hydride donors. Asymmetric resolution: Dynamic resolution, Dynamic kinetic resolution and Dynamic Thermodynamic resolution.

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

**Reference Books: PCH 1802: Organic Chemistry:(Theory)**

1. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March, 6<sup>th</sup> Edition, John Wiley.
2. Carbenes, nitrenes and arynes, T.L. Gilchrist and C.W. Rees.
3. Guidebook to Mechanism in Organic Chemistry by Peter Sykes, 6th Edition, Prentice Hall.
4. Advanced Organic Chemistry Part A: Structure and Mechanism and Part B: Reaction and synthesis, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer.
5. Advanced Organic Chemistry Part B: Structure and Mechanism and Part B: Reaction and synthesis, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer.
6. Organic Chemistry, Jonathan Clayden, Nick Greeves, Stuart Warren, 1st Edition, Oxford University Press.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, 3rd Edition, Blackie Academic and Professional.
8. Stereo Chemistry, P.S. Kalsi, New Age Publications.
9. Reagents in Organic Synthesis- Fieser and Fieser, John Wiley.
10. Stereochemistry of Organic Compounds, Ernest L. Eliel, Samuel H. Wilen, Wiley- Blackwell.
11. Organic Chemistry, T.W. Graham Solomons and Graig B. Frymes, John Wiley and Sons.
12. Organic Chemistry, F. A. Carey, McGraw Hill Edition.
13. Dynamic Stereochemistry of Chiral Compounds: Principles and Applications, Christian Wolf, RSC publishing.
14. Organic Chemistry Vol 1-2 I.L.Finar 5<sup>th</sup> edition, ELBS.
15. Organic Reaction mechanism, Third edition, V. K. Ahluwalia, Rakeshkumar Parashar, Narosa Publishing house New Delhi.

## Semester I

### CORE Paper: Physical Chemistry (Theory)

Course Code: PCH 1803

No. of Credits: 04

Learning Hours: 60 hrs (70 Marks)

### Course Overview & Course Objectives

The main objective of the course will be to enhance the understanding and knowledge of Physical Chemistry without an obscuring mathematical screen.

By the end of the paper, a student will be able to:

- a. Understand the details and utility of the entire topics in physical chemistry, separately as well as in context to one another.
- b. The long major areas of study such as thermodynamics and kinetics are so taught, such that students are able to move on to more advanced studies.

Thus, the knowledge from the course can help in the following:

The other topics, like Solid State and Surface Chemistry are so decided upon so that students can increase their conceptual base in this subject which will be needed by students in their pursuit of research in other allied branches of chemistry.

### **Course Content**

#### **Unit-1: Chemical thermodynamics (15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Chemical thermodynamics]

Experimental verification of third law of thermodynamics, entropy correction for real gases, partial molar quantities and their determination, Gibbs-Duhem equation, chemical potential, chemical potential of ideal gases and solutions, Raoult's law, real solutions, free energy and solutions, activity and activity coefficients, fugacity of gases and liquids and methods of its determination. Non equilibrium thermodynamics-basic concepts.

#### **Unit-2: Chemical Kinetics (15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Chemical Kinetics]

Unimolecular reactions, chain reactions and branched chain reactions, explosion limits, chain reaction between hydrogen and bromine, theory of absolute reaction rates, Kinetics of fast reaction and some experimental techniques for studying fast reactions like NMR, Mass Spectroscopy, Gas chromatography, Flow method and Flash photolysis method.

#### **Unit-3: Solid state chemistry (15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Solid state chemistry]

Bonding in solids and electronic structure in solids, bond theory-metals, semiconductors and insulators, defects in crystals, calculation of Schottky and Frenkel defects using statistical method, non-stoichiometry –FeO (wustite), solid electrolytes, diffusion in solids- Fick's laws, mechanism of diffusion, electrical conductivity in solids, super conductivity, perovskites.

#### **Unit-4: Surface chemistry (15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Surface chemistry]

Physical and chemical adsorption, BET equation, heat of adsorption and its measurement by Calorimetric and Clausius Clapeyron equation methods, determination of surface area of adsorbents by BET method, surface tension and adsorption from solutions, Gibbs' adsorption equation, micellisation and critical micellar concentration (cmc).

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books

and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

### **Reference books: PCH 1803: Physical Chemistry (Theory)**

1. Physical chemistry by W. J. Moore, 5<sup>th</sup> edition, orient longman private ltd.
2. Textbook of physical chemistry by S. Glasstone, D. Van Nostrand company, inc., 1946.
3. Textbook of physical chemistry by Peter Atkins Julio de and Paula , 9<sup>th</sup> edition, oxford press.
4. Advanced physical chemistry by Gurdeep Raj 35<sup>th</sup> revised edition, Goel publishing house.
5. Advanced physical chemistry by J .N. Gurtu, A. Gurtu, 11<sup>th</sup> edition , Pragati prakashan.
6. Thermodynamics for chemists by S. Glasstone, Read Books, 2007.
7. Physical chemistry by S. Castellan, 3<sup>rd</sup> edition, Pearson Custom Publishing.
8. Thermodynamics of non equilibrium processes- Karapitaneh
9. Chemical Kinetics by Laidler, 3<sup>rd</sup> edition, Pearson Education India.
10. Chemical Kinetics – Frost and Pearson
11. Principles of the Solid State by H.V. Keer, 2<sup>nd</sup> edition ,New Age Internation (P) Ltd.
12. Solid state chemistry by Hannay,Prentice-hall,1967.
13. Introduction to Solids by L. Azaroff, 1<sup>st</sup> edition, McGraw Hill Education India Pvt Ltd.
14. Physical Chemistry of Surfaces by A.W.Adamson,6<sup>th</sup> eddition, Wiley-Interscience.
15. Surface chemistry – Osipov
16. Solid State Chemistry and its Applications by Anthony R West, 2<sup>nd</sup> editon 2014,Wiley.
17. Chemical Thermodynamics: Classical, Statistical and Irreversible by Rajaram & Kuriakose, S Chand, 2<sup>nd</sup> edition.

### **Semester I**

#### **CORE Paper: Analytical Chemistry (Theory)**

**Course Code: PCH 1804**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

#### **Course Overview & Course Objectives**

The main objective of the course will be to enhance the understanding and knowledge of Analytical Chemistry, for students studying , any branch of chemistry .

By the end of the paper, a student will be able to:

- a. Understand the very important role of an analytical chemist in all branches of chemistry.
- b. Know and study the work-up required by all samples before they can be subjected to analysis and also learn about the various types of analysis.
- c. Will study about the most widely employed technique i.e. spectrophotometry and its application in analytical chemistry and other branches of chemistry.
- d. Will study about thermal methods of analysis which is able to provide valuable analytical data.



Thus, the knowledge from the course can help in the following:

All students, of all branches whether organic or inorganic will be able to incorporate this knowledge, in their pursuit of research in their different fields.

### **Course Content**

#### **Unit-1: Analytical objectives, sampling and calibration methods (15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Analytical objectives, sampling and calibration methods]

Scope of analytical science and its literature, sampling and sample preparation, general steps in chemical analysis, calibration and classification of glassware, validation of analytical methods, finding the best straight line-least square regression, correlation coefficient, calibration curves, standard addition technique internal standard method. Numericals based on chemical concentrations.

#### **Unit-2: Fundamentals of spectrophotometry (15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Fundamentals of spectrophotometry]

Properties of light, absorption of light, interaction of light with matter and origin of spectra, spectrophotometer-instrumentation of single and double beam, Beers Law-its use, limitation and numericals, photometric accuracy.

#### **Unit-3: Applications of spectrophotometry (15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Applications of spectrophotometry]

Analysis of mixture, measurement of equilibrium constant, Scatchard Plot, Stoichiometry determination-method of continuous variation-Jobbs Plot, Photometric titrations.

#### **Unit-4: Thermal methods of analysis (15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Thermal methods of analysis]

Principle, instrumentation and applications of Thermo Gravimetric Analysis (TGA), Differential thermal analysis(DTA) and Differential Scanning Calorimetry (DSC).

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

**Reference books: PCH1804: Analytical Chemistry (Theory)**

1. Quantitative Chemical Analysis, by Daniel C. Harris, 5<sup>th</sup> Edition, W.H. Freeman and Company, New York.
2. Analytical Chemistry, by Gary D. Christian, 6<sup>th</sup> Edition, John Wiley and Sons Inc. New Jersey.
3. Principles of Instrumental Analysis, by Douglas A. Skoog, 3<sup>rd</sup> Edition, Holt- Saunders International Edition.
4. Instrumental Methods of Chemical Analysis, by Galen W. Ewing, 4<sup>th</sup> Edition, International Student Edition.

**Semester I****Paper: Inorganic Chemistry and Organic Chemistry (Practicals)****Course Code: PCH 1805L****No. of Credits: 04****Learning Hours: 60 hrs (70 Marks)****Course: PCH 1805L (A) Inorganic Chemistry (Practicals)****Course Content**

1. Semi-microqualitative analysis of 15 mixtures, each having six radicals including less familiar elements (Mo, W, Li, Th, V, Zr, Ce, Be, Ti) and one insoluble compounds.
2. Green Preparations:-
  - A) Preparation of Manganese (III) acetylacetonate,  $\text{Mn}(\text{acac})_3$  or  $\text{Mn}(\text{C}_5\text{H}_7\text{O}_2)_3$ .
  - B) of Iron (III) acetylacetonate,  $\text{Fe}(\text{acac})_3$  or  $\text{Fe}(\text{C}_5\text{H}_7\text{O}_2)_3$

**Teaching methodologies Preparation:** Practical work, problem solving, and group discussion etc.

**References books: PCH1805L (A): Inorganic Chemistry (Practicals)**

1. Vogel's Qualitative Inorganic Analysis, Revised by G Svehla, Sixth Edition, Longman, 1987.
2. Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST.

**Course: PCH 1805L (B) Organic Chemistry (Practicals)****Course Content****1. Preparation of organic compounds: Single Stage Preparations:**

- a. Preparation of 1-Phenyl-3-methyl-5 pyrazolone from acetoacetic ester.
- b. Preparation of Dibenzylidene acetone from Benzaldehyde.
- c. Preparation of o-Chlorobenzoic acid from o-amino benzoic acid.

- d. Preparation of 2,4-Dinitroanisole from Anisole
- e. Preparation of Phthalimide from phthalic acid.
- f. Preparation of Para Red
- g. Preparation of methyl Orange.
- h. Preparation of Benzo triazole from o-Phenylene diamine
- i. Preparation of 1,2,3,4 tetrahydrocarbazole from phenyl hydrazine. (Fisher Indole synthesis)
- j. Preparation of p-Bromo acetanilide from acetanilide (Green route)

## 2. Quantitative Estimations:

- a. Estimation of ester + acid
- b. Estimation of Formaldehyde
- c. Estimation of glycine
- d. Estimation of amide + acid

**Teaching methodologies:** Practical work, problem solving, and group discussion etc.

## References books: PCH 1805L (B): Organic Chemistry (Practicals)

1. A text book of practical organic chemistry – A. I. Vogel
2. Practical organic Chemistry – Mann and Saunders
3. A handbook of quantitative and qualitative analysis – H. T. Clarke
4. Comprehensive Practical Organic Chemistry : Qualitative Analysis V K Ahluwalia & S. Dhingra.
5. Comprehensive Practical Organic Chemistry : Preparations and Quantitative Analysis V K Ahluwalia& R. Aggarwal Universities Press.
6. An Advance Course in practical Chemistry, A K. Nad, B. Mahapatra and A. Ghoshal.

## Semester I

### Paper: Physical Chemistry and Analytical Chemistry (Practicals)

**Course Code: PCH 1806L**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

### Course: PCH 1806L (A) Physical Chemistry (Practicals)

#### Course Content

##### 1. Conductometry

- a. To determine on centration of HCl and NH<sub>4</sub>Cl in a given solution conductometrically (requirements: 0.05N HCl, 0.5 N NH<sub>4</sub>Cl, 0.5 N NaOH)
- b. Estimate the concentration of H<sub>2</sub>SO<sub>4</sub>, CH<sub>3</sub>COOH and C<sub>12</sub>H<sub>10</sub>O<sub>4</sub> 5 H<sub>2</sub>O in a given solution conductometrically. (0.005M all against 0.05N NaOH)

## 2. Potentiometry

- To construct the calibration curve for quinhydrone electrode and hence the standard oxidation potential of quinhydrone electrode. (0.2N  $\text{CH}_3\text{COONa}$ , 0.2N  $\text{CH}_3\text{COOH}$ )
- Solubility product of silver halides.

## 3. pH metry

- To determine the amount of Aspirin in a given solution.(aspirin,0.1N alcoholic KOH, glass and calomel electrodes)
- Titration of mixture of bases ( $\text{Na}_2\text{CO}_3$  &  $\text{NaHCO}_3$ ) with standard HCl and find the concentration of bases.

## 4. Adsorption and kinetics

- To study the rate of acid catalysed ionization of acetone in presence of excess acid and acetone at room temp. (requirement: acetone, iodine, sulfuric acid sodium acetate, 0.01sodium thiosulphate, starch)
- To determine the autocatalytic reaction between  $\text{KMnO}_4$  and oxalic acid.  
(Requirements:0.1M  $\text{H}_2\text{C}_2\text{O}_4$ , 10%KI , 0.01M  $\text{Na}_2\text{S}_2\text{O}_3$ , 0.02M  $\text{KMnO}_4$ ,0.2M  $\text{MnSO}_4$ , 1% starch, 1.0 M  $\text{H}_2\text{SO}_4$ )

## 5. Distribution method

- Distribution of HAC between  $\text{H}_2\text{O}$  and  $\text{CHCl}_3 / \text{CCl}_4$ .
- Distribution of  $\text{I}_2$  between  $\text{H}_2\text{O}$  and  $\text{CCl}_4$ .

**Teaching methodologies:** Practical work, problem solving, and group discussion etc.

### References books: PCH1806L (A): Physical Chemistry (Practicals)

- Advanced Practical Physical Chemistry By J.B.Yadav, 32<sup>nd</sup> edition Krishna publication.
- Practicals in physical chemistry by P.S.Sindhu, Macmillan 2005.
- Experimental physical chemistry by R.C.Das, B.Behera Tata McGraw-Hill, 1983.
- Experimental Physical Chemistry by Athwale , Mathur and Parul, 1<sup>st</sup> edition reprint 2011, New Age International (P) Ltd.

## Semester I

### Course: PCH 1806L (B) Analytical Chemistry (Practicals)

#### Course Content

- Calibration of glass wares and balance.
- Determination of % age purity of given sample of Isoniacid.
- Determination of % age of Asprin in the given tablet.
- Determination of available chlorine in bleaching powder.

5. Determination of vitamin C in orange juice/amla.
6. Determination of acetic acid in vinegar.
7. Determination of sodium carbonate and sodium bicarbonate in washing soda.
8. Determination of ascorbic acid in vitamin C tablets.
9. Determination of % age purity of given sample of Analgin tablet.
10. Determination of calcium and magnesium in water sample.
11. Determination of sulphate in water sample.
12. Determination of chloride in water sample.

**Teaching methodologies:** Practical work, problem solving, and group discussion etc.

**References books: PCH 1806L (B): Analytical Chemistry (Practicals)**

1. Analytical Chemistry Practice, John H. Kennedy, Saunders College Publishing, Second Edition 1990.
2. Vogels Textbook of Quantitative Chemical Analysis, 6th Edition, 2002.

## Semester II Overview

Sub. code	Course	Instructi on Hrs/wee k	Internal Assesse nt Marks	Max Marks Semeste r Exams	Duratio n of Semeste r Exam (Hrs)	Credi t
<b>THEORY</b>						
PCH 2801	Inorganic Chemistry	4	30	70	3	4
PCH 2802	Organic Chemistry	4	30	70	3	4
PCH 2803	Physical Chemistry	4	30	70	3	4
PCH 2804	Analytical techniques	4	30	70	3	4
<b>PRACTICALS</b>						
PCH 2805L	Inorganic Chemistry Lab-I	3	30	70	3	4
	Organic Chemistry Lab-I	3			3	
PCH 2806L	Physical Chemistry Lab-I	3	30	70	3	4
	Analytical Chemistry Lab-I	3			3	
<b>Total</b>		<b>28</b>	<b>180</b>	<b>420</b>		<b>24</b>

Note:- Semester -I and Semester-II syllabus is common for all specializations to be selected by the students for final year i.e. Inorganic, Organic, Physical and Analytical. At present St. Xavier's College offers only Organic Chemistry as a specialization in the final year of M Sc Chemistry.

## Semester II

## **CORE Paper: Inorganic Chemistry (Theory)**

**Course Code: PCH 2801**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

### **Course Overview & Course Objectives**

The main objective of the course will be to enhance the understanding and knowledge of Inorganic Chemistry, for students studying, any branch of chemistry.

By the end of the paper, a student will be able to:

- Understand the important aspects of Chemical Bonding and Atomic Structure
- Know and study the applications Symmetry and Group Theory
- Understand the important aspects of Organometallic Compounds
- Know and study Reaction Mechanism in inorganic chemistry.

Thus, the knowledge from the course can help in the following:

- Finally, all students, of all branches whether organic or inorganic will be able to incorporate this knowledge, in their pursuit of research in their different fields.

### **Course Content**

#### **Unit-1: Chemical Bonding (15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to VSEPR theory and Chemical Bonding]

VSEPR, Walsh diagrams(tri atomic molecules), Bent rule and Simple Huckel theory of linear conjugated systems, simple Huckel theory of the cyclic conjugated system and aromaticity, self-consistent field method, valence state ionization potentials, Band theory of solids, Fermi level, electrical properties, insulators, semiconductors and superconductors (properties).

#### **Unit-2: Application of symmetry (15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to symmetry and IR and Raman spectra]

Application of symmetry to hybrid orbital, molecular orbitals, hybridization schemes for  $\sigma$  orbitals,  $\pi$  bonding and molecular orbital for  $AB_n$  type of molecules.

Application of symmetry to molecular vibrations, interpretation of IR and Raman spectral data.

#### **Unit-3: Organometallic Compounds (15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Organometallic Compounds]

Organometallic compounds of transition elements, stability of metal carbon bond in complexes. Synthesis, uses and structure of organometallic compounds of  $\pi$  bonding organic ligands, 2-

electron ligands, olefinic and acetylinic complexes, compound with 3 electron ligand – allylic complexes, compounds. With 4- electron ligands butadiene complexes,  $n_4$  complexes of cyclopentadiene, compounds with 5 electron ligands – cyclopentadienyl, compounds with 6 electron ligands,  $n_6$  complexes of benzene and its derivatives. Role of organometallic compounds in catalytic reaction.

#### **Unit-4: Reaction Mechanism**

**(15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Inorganic Reaction Mechanism]

Mechanism of substitution reaction in square planar complexes. Kinetics of substitution reaction of platinum (II) complexes.

Effect of leaving group, effect of charge, steric effect, solvent effect, effect of nucleophile, effect of temperature and other effects.

Oxidation-Reduction reaction, electron transfer, tunnelling effect, Marcus –Hush theory, one and two electron transfer inner sphere and outer sphere, effect of ions on rate, electron transfer through extended bridges, unstable oxidation states, hydrated electron.

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

#### **References books: PCH 2801: Inorganic Chemistry (Theory)**

1. Introduction to Quantum Chemistry, A. K. Chandra, Tata MacGraw Hill
2. Quantum Chemistry, Ira N. Levine, Prentice Hall
3. Quantum Chemistry by R. K. Prasad, New Age International Publishers (1985)
4. D. A. McQuarrie Quantum Chemistry, OUP 1983
5. M. W. Hanna, Quantum Mechanics in Chemistry, The Benjamin Pub.
6. Lectures on Chemical Bonding and Quantum Chemistry, S. N. Datta, A Prism Book
7. Group theory and symmetry in chemistry, L. H. Hall(McGraw Hill)
8. Coulson's Valence, R. McWeeny, ELBS
9. F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern 2nd Edn.1992
10. V. Ramkrishnan& M. S. Gopinadhan, Group theory in Chemistry Vishal Pub.1996.
11. Inorganic Chemistry, Third Edition, Alan G. Sharpe
12. Theoretical Inorganic Chemistry, M. C. Day, J. Shellin
13. Chemistry, Fifth Edition, John E. McMurry, Robert C. Fay
14. An Introduction to Theoretical Chemistry, Jack Simons, Cambridge
15. Progress in inorganic Chemistry, Vols 18 and 38 ed. J. J. Lippard, Wiley
16. Mechanism of Inorganic Reactions, F. Basolo and R. G. Persons, Wiley Pub



17. Reaction Mechanism of Coordination Compounds, C. H. Langford and H. B. Gray
18. Inorganic Reaction Mechanisms, M. L. Tobe, Nelson Pub
19. Inorganic Chemistry, K. F. Purcell and J. C. Kotz.
20. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Bers
21. Mehrotra R. C. and Singh A. Organo Metallic Chemistry, Willey Eastern Ltd., New Delhi
22. Coates G. E. Green MIH Wade, K and Aylett B. J. Organo Metallic Comounds Chapman and Hall, London.

## Semester –II

### CORE Paper: Organic Chemistry (Theory)

Course Code: PCH 2802

No. of Credits: 04

Learning Hours: 60 hrs (70 Marks)

### Course Overview & Course Objectives

The main objective of the course will be to enhance the understanding and knowledge of organic chemistry.

By the end of the paper, a student will be able to:

- a. Understand the details of Application Redox and reagents in organic synthesis
- b. The chemistry of Photochemistry and Heterocyclic compounds
- c. Understand the importance of Organic Name reactions
- d. Understand the details of various aspects of Reagents in organic synthesis.

Thus, the knowledge from the course can help in the following:

This content can help students to increase their conceptual base and understanding in these topics which will be needed by students in their pursuit of research in other allied branches of chemistry.

### Course Content

#### Unit-1: Application Redox and reagents in organic synthesis. (15L) [14Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Oxidation and reduction]

- a. Oxidizing agents, Reducing agents and Mechanistic explanation of oxidation and reduction with example. Oxidation with Manganese,  $\text{KMnO}_4$ , Chromium, Peracid, Peroxide, Dimethyl dioxarane  $\text{SeO}_2$ , NBS, DDQ, Chloranil and Oppenauer oxidation.
- b. Reduction:
  - (i) Reduction with Hydride transfer reagents like  $\text{LiAlH}_4$ ,  $\text{NaBH}_4$ , Diborane.
  - (ii) Reduction by Dissolving metals Zn, Li, Na.
  - (iii) Birch reduction and catalytic reduction.

#### Unit – 2

(15L) [14Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Photochemistry and Heterocyclic compounds]

### 1. Photochemistry:

- A) Photochemical reactions: Principles of energy transfer, electronic excitation and molecular orbital view of excitation, excited states and excitation and molecular orbital view of excitation, excited states and fate of excited molecules (modified Jablonski diagram), Photosensitization.
- B) Photochemistry of carbonyl compounds: Representation of excited states of ketones, photo reduction Norrish type I & II reactions, Reactions of cyclic Ketone, oxetane formation (Paterno-Buchi reaction)
- C) Di- $\pi$  methane rearrangement, Dienone photochemistry, cis-trans isomerisation and photochemistry of conjugated olefins.

### 2. Chemistry of Heterocycles

- A) Nomenclature of heterocycles: Few examples of systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles. General chemical behavior of following aromatic heterocycles: their synthesis and important applications. (Three examples each).
- B) Five-membered and benzo fused five member heterocycles : Oxazole, Isoxazole, Thiazole, Pyrazole, Imidazole, Benzothiazole and Benzimidazole.
- C) Six membered and benzofused six membered heterocycles : Pyrazine, Pyridazine, Pyrimidine, Cinnoline, Quinazoline, Quinoxaline, Phenoxaline.

### Unit-3: Name reactions:

(15L) [14Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Name reactions]

General nature, method, mechanism and synthetic applications of the following named organic reactions:

- |                            |  |
|----------------------------|--|
| (i) Suzuki reaction        | (ii) Buchwald Hartwing reaction (cross coupling) |
| (iii) Sonogashira coupling | (iv) Vilsmeier-Haack reaction                    |
| (iv) Mitsunobu reaction    | (vi) Stobbe condensation                         |
| (vii) Jones oxidation      | (viii) Swern oxidation reaction                  |
| (ix) Michael addition      | (x) Dickmann reaction                            |
| (xi) Knoevenagel reaction  | (xii) Darzen's glycidic ester synthesis          |
| (xi) Mannich reaction      | (xiv) Wittig reaction                            |

**Unit-4: Reagents in organic synthesis:****(15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Reagents in organic synthesis]

Mechanism selectivity and utility of following reagents:

- |  |  |
|--|--|
| (i) Gilman's reagent-Lithium dimethylcuprate   | (ii) Lithium diisopropylamide (LDA)    |
| (iii) Dicyclohexylcarbodiimide (DCC)   | (iv) 1,3 – Dithiane (Umpolung reagent) |
| (v) Dess- Martin periodinane   | (vi) Bakers yeast                      |
| (vii) Diisobutylauminiumhydride(DIBAL –H)  |  |
| (viii) Sodium cyanoborohydride( $\text{NaBH}_3(\text{CN})$ )                               | (ix) Grignard reagents                 |
| (x) Sodium borohydride   | (xi) DDQ                               |
| (xii) n-Butyl lithium  |  |
| (xiii) Phase transfer catalysis : Quaternary ammonium and phosphonium salts, crown ethers. |  |

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

**References books: PCH 2802: Organic Chemistry (Theory)**

1. Modern Synthetic Reactions, H.O.House, W.A. Benjamin.
2. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, 3rd Edition, Blackie  
a. Academic and Professional.
3. Introductory Photochemistry, A. Cox and T. Camp, McGraw Hill.
4. Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.
5. Organic Photochemistry, J. Coxon and B. Halton, 2nd Edition, Cambridge University Press.
6. Strategic Applications of Named Reactions in Organic Synthesis, Laszlo Kurti and Barbara Czak, 1st Edition, Academic Press.
7. Name Reactions and Reagents in Organic Synthesis, Bradford P. Mundy, Michael G. Ellerd, Frank G. Favaloro, 2nd Edition, Wiley – Interscience.
8. Name Reactions. A Collection of Detailed Reaction Mechanisms., Jie Jack Li, 3<sup>rd</sup> Edition Springer.
9. Heterocyclic Chemistry, volume 1-3, R.R. Gupta, M. Kumar and V. Gupta, Springer- Verlag.
10. Heterocyclic Chemistry, J.A. Joule, K.Mills, and G.F. Smith, 3rd Edition, Chapman and Hall.
11. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technical.
12. Contemporary Heterocyclic Chemistry, G.R. Nikome and W.W. Poudler, Wiley.
13. Comprehensive Heterocyclic Chemistry, A.R. Kartizky, and C.W. Rees.
14. Encyclopedia of Reagents for Organic Synthesis, Leo A. Paquette, David Crich and Phillip L. Fuchs, John Wiley and Sons Inc.
15. Organic Chemistry, T.W. Graham Solomons and Graig B. Frymes, John Wiley and Sons.

16. General Organic Chemistry Sachin Kumar Ghose, New Central book agency.
17. Guidebook to Mechanism in Organic Chemistry by Peter Sykes, 6th Edition, Prentice Hall.
18. Advanced Organic Chemistry Part A: Structure and Mechanism and Part B: Reaction and synthesis, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer.
19. Organic Chemistry Vol 1-2 I.L. Finar 5th edition, ELBS.
20. Advance organic chemistry by Jerry March
21. Advance organic chemistry by Carey and Sundberg,
22. Advance organic chemistry by Francis A. Carey.

## **Semester –II**

### **CORE Paper: Physical Chemistry (Theory)**

**Course Code: PCH 2803**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

### **Course Overview & Course Objectives**

The main objective of the course will be to enhance the understanding and knowledge of Physical Chemistry without an obscuring mathematical screen.

By the end of the paper, a student will be able to :

- a. Understand the details and utility of the entire topics in physical chemistry, separately as well as in context to one another.
- b. The long major areas of study such as Statistical thermodynamics and Nuclear chemistry are so taught, such that students are able to move on to more advanced studies.

Thus, the knowledge from the course can help in the following:

The other topics, like Polymer chemistry and Electrochemistry are so decided upon so that students can increase their conceptual base in this subject which will be needed by students in their pursuit of research in other allied branches of chemistry.

### **Course Content**

#### **Unit-1: Statistical thermodynamics**

**(15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Statistical thermodynamics]

Concepts of distribution of molecules, microstate and macro state. Ensemble averaging, Canonical, grand canonical and microcanonical ensembles, Maxwell-Boltzman distribution laws (using Lagrange's method of undetermined multipliers). Fermi-Dirac statistics – distribution law and Bose-Einstein statistics – distribution law.

Partition functions – translational, rotational, vibrational and electronic partition

**Unit-2: Nuclear chemistry** (15L) [14Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Nuclear chemistry]

Nuclear properties-nuclear radius, coulombic and nuclear potential radius, nuclear spin and angular momentum, magnetic moment, nuclear binding energy, nuclear models-shell model, liquid drop model, Fermi gas model, collective model, radioactive decay, nuclear reactions, evaporation, spallation, fragmentation, fission and fusion reactions, accelerators, reaction cross section, use of radioisotopes as tracers.

**Unit-3: Polymer chemistry** (15L) [14Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Polymer chemistry]

Kinetics and mechanism of polymer processes, criteria of polymer solubility, thermodynamics of polymer solutions, polymer characterization, molecular weight of polymer (number average and weight average), methods of molecular weight determination, properties of polymers and applications.

**Unit-4: Electrochemistry** (15L) [14Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Electrochemistry]

Sign convention-American, European and IUPAC; Polarization ,demonstration of polarization , elimination of polarization ,Decomposition Potential-Factors ,applications and measurement of Decomposition potential and Overvoltage and factors affecting overvoltage, basic principle of polarography, origin of different types of current; Ilkovic equation. polarographic wave equation, Importance of  $E_{1/2}$  in polarography ,Dependence of  $E_{1/2}$  on pH and complexing agents (derivation),Pilot ion method and standard addition method to determine concentration.

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

**Reference books: PCH 2803: Physical Chemistry (Theory)**

1. Physical chemistry by W.J.Moore, 5<sup>th</sup> edition, orient longman private ltd.
2. Textbook of physical chemistry by S. Glasstone, D. Van Nostrand company, inc., 1946.
3. Textbook of physical chemistry by Peter Atkins Julio de and Paula , 9<sup>th</sup> edition, oxford press.
4. Advanced physical chemistry by Gurdeep Raj 35<sup>th</sup> revised edition, Goel publishing house.
5. Advanced physical chemistry by J.N.Gurtu, A.Gurtu, 11<sup>th</sup> edition , Pragati prakashan.

6. Statistical thermodynamics by M.C.Gupta ,revised 2<sup>nd</sup> edition, New Age International publishers
7. Thermodynamics,statistical thermodynamics and kinetics by T.Engle and P.Reid, Pearson India.
8. Thermodynamics: A core course , by Srivastava,Saha and jain, 3<sup>rd</sup> edition,Prentice-hall of India
9. Polymer science by Gowariker, New Age International, reprint 1986.
10. Textbook of Polymer Science By Fred W. Billmeyer Jr., 3rd Edition edition (2 May 1984), Wiley-Blackwell.
11. Principles of Polymer Science, 2<sup>nd</sup> edition by Bahadur & Sastry, Alpha Science.
12. Polymer science & technology by Fried, 3<sup>rd</sup> edition, Printece-Hall.
13. Polymer Chemistry: An Introduction by Malcolm P. Stevens, 3<sup>rd</sup> edition, Addison-Wesley Publishing Company.
14. Essentials of Nuclear Chemistry by Arnikaar, New Age Internation
15. Nuclear and radio chemistry by J.W. Kannedy, G.Friedlander, 3<sup>rd</sup> edition, Wiley.
16. Modern Electrochemistry by Bockris and Reddy

**CORE Paper: Analytical Chemistry (Theory)**

**Course Code: PCH 2804**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

**Course Overview & Course Objectives**

The main objective of the course will be to enhance the understanding and knowledge of Analytical Chemistry, for students studying, any branch of chemistry.

By the end of the paper, a student will be able to:

- a. Understand the very important role of an analytical chemist in all branches of chemistry.
- b. Know and study the work-up required by all samples before they can be subjected to analysis and also learn about the various types of analysis.
- c. Will study about the most widely employed technique i.e. Principles of chromatography and its application in analytical chemistry and other branches of chemistry.
- d. Will study about Electro-Analytical methods of analysis which is able to provide valuable analytical data. Thus, the knowledge from the course can help in the following:

All students, of all branches whether organic or inorganic will be able to incorporate this knowledge, in their pursuit of research in their different fields.

**Course Content**

**Unit-1: Sample Preparation Techniques**

**(15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Sample Preparation Techniques]

Liquid-liquid extraction/solvent extraction-partition coefficient, distribution ratio and percent extraction. Solvent extraction of metal ions-ion association complexes and metal chelates, multiple batch extraction, Craig's counter-current distribution. Accelerated and Microwave assisted extraction, protein precipitation and solid phase extraction (SPE).

### **Unit -2: Basic Principles of chromatography (15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Basic Principles of chromatography]

Chromatographic Methods Principles of chromatography, classification of chromatographic techniques based on mechanism of retention, configuration, mobile and stationary phase.

Importance and meaning of terms –Partition Ratio, Retention Time and Dead Time, Capacity Factor and Selectivity Factor, Efficiency of separation- plate theory (theoretical plate concept) and rate theory (Van Deemter equation).

### **Unit-3: Specialized chromatographic techniques (15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Basic Principles of chromatography and Specialized chromatographic]

Principles ,instrumentation and applications of Gas Chromatography, HPLC, HPTLC and Ion exchange chromatography .

### **Unit-4: Electro-Analytical Chemistry (15L) [14Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Electro-Analytical Chemistry]

pH measurement with glass electrode, working of glass electrode, mechanism of pH measurement, calibration of glass electrode, errors in pH measurement. Classification, principle, properties and design of ion selective membrane electrodes- Glass electrodes for ions other than  $H^+$ , Solid precipitate electrode and single crystal electrode, Liquid ion exchange electrode, ion molecular sieve electrodes. Ion, Gas-sensing probes and enzyme substrate electrodes.

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

### **Reference books: PCH 2804: Analytical Chemistry (Theory)**

1. Quantitative Chemical Analysis, by Daniel C. Harris, 5<sup>th</sup> Edition, W.H. Freeman and Company, New York.

- Analytical Chemistry, by Gary D. Christian, 6<sup>th</sup> Edition, John Wiley and Sons Inc. New Jersey.
- A Practical handbook of preparative HPLC by Donald Wellings, Elsevier, 2006.
- Ion-pair chromatography: Theory and Biological and Pharmaceutical Applications (Chromatographic Science), Milton Hearn (editor), Marcel and Dekker Inc. (1985).
- Practical Aspects of Gas Chromatography/Mass Spectroscopy by Gordon M. Message, John Wiley & Sons, 1984.
- Modern Practice of Gas Chromatography by Robert L. Grob and Eugene F. Barry, 3<sup>rd</sup> edition, Wiley-Interscience, 1995.
- Basic Gas Chromatography by Harold M. McNair, James M. Miller, John Wiley and Sons, 2008.
- Analytical gas Chromatography by Walter Jennings, Eric Mittlefehldt and Philip Stremple, second edition, Elsevier Science, 1997.
- Modern HPLC for practicing scientists by Michael W. Dong, Wiley Interscience, 2006.

**Paper: Inorganic Chemistry and Organic Chemistry (Practicals)**

**Course Code: PCH 2805L**

**No. of Credits: 04**

**Learning Hours: 60 (70 Marks)**

**Course: PCH 2805L (A) Inorganic Chemistry (practicals)**

**Course Content**

- Preparation and determination of purity of double and complex salts. At least seven preparations should be done.
- Colourimetric estimation of any four out of Cu, Mn, NO<sub>2</sub>, Ni, P, Fe, V, Ti, Cr, Co.

**Teaching methodologies:** Practical work, problem solving and group discussion etc.

**References books: PCH 2805L (A) : Inorganic Chemistry(Practicals)**

- Vogel's Textbook of Quantitative Chemical Analysis, 6th Edition, 2002.
- Advanced Practical Inorganic Chemistry, Gurdeepraj, Goel Publishing House, 2001.
- An Advanced Course in Practical Chemistry, A.K. Nad, B. Mahapatra, A. Ghosal, New Central Book Agency, 2004

**Course: PCH 2805L (B) Organic Chemistry (practicals)**

**Course Content**

Mixture analysis: ternary mixture to be given. (S+S+S )or ( L+L+L ). Type determination. Separation by physical and chemical methods. (both permitted in case of liquids).

**Teaching methodologies:** Practical work, problem solving and group discussion etc.



**References books: PCH 2805L(B): Organic Chemistry (Practicals)**

1. A text book of practical organic chemistry – A. I. Vogel
2. Practical organic Chemistry – Mann and Saunders
3. A handbook of quantitative and qualitative analysis – H. T. Clarke
4. Comprehensive Practical Organic Chemistry : Qualitative Analysis V K Ahluwalia & S. Dhingra.
5. Comprehensive Practical Organic Chemistry : Preparations and Quantitative Analysis, V K Ahluwalia & R. Aggarwal Universities Press.
6. An Advance Course in practical Chemistry, A K. Nad, B. Mahapatra and A. Ghoshal.

**Paper: Physical Chemistry and Analytical Chemistry (Practicals)****Course Code: PCH 2806L****No. of Credits: 04****Learning Hours: 60 (70 Marks)****Course: PCH 2806L (A) Physical Chemistry (practicals)****Course Content****1. Conductometry**

- a. Test of validity of Ostwald's dilution law and determination of dissociation constant of weak electrolyte like  $\text{CH}_3\text{COOH}$  &  $\text{ClCH}_2\text{COOH}$
- b. Verification of Debye-Huckel-Onsager's equation in case of strong electrolytes like HCl, KCl, NaCl.

**2. Potentiometry**

- a. Titration of dibasic acid like malonic, oxalic, succinic acid with NaOH and find the dissociation constant of acid.
- b. Precipitation titration → Titration of halides with  $\text{AgNO}_3$ .
- c. Redox titration Ferrous ammonium sulfate –  $\text{KMnO}_4$ ,  $\text{K}_2\text{Cr}_2\text{O}_7$ .

**3. pH metry**

- a. Determination of dissociation constant of weak acid like acetic and monochloroacetic acid
- b. To titrate phosphoric acid solution against alkali and to calculate the first, second and third ionization constant of it. (0.05M phosphoric acid, 10% neutral  $\text{CaCl}_2$ , 0.5N NaOH)

**4. Kinetics**

- a. Determination of the effect of (a) Change of temperature (b) Change of concentration of

reactant and catalyst and (c) Ionic strength of the media on the velocity constant of an acid hydrolysis of an ester.

- b. Determination of order of reaction between  $K_2S_2O_8$  and KI by a fractional change method

#### **5. Distribution method**

- a. Determination of the formula of the complex formed between cupric ion and ammonia by distribution method.

**Teaching methodologies:** Practical work, problem solving and group discussion etc.

#### **References books: PCH 2806L (A): Physical Chemistry (Practicals)**

1. Practical physical chemistry –J.B.Yadav
2. Practicals in physical chemistry – P.S.Sindhu
3. Experimental physical chemistry – R.C.Das, B.Behera
4. Experiments in physical chemistry- P.H.Parsania, F. Karia

#### **Course: PCH 2806L (B): Analytical Chemistry (practicals)**

##### **Course Content**

1. Determination of saponification value of oil.
2. Determination of iodine value of oil.
3. Determination of iron by chloride extraction by solvent extraction process.
4. Determination of dissolved oxygen.
5. Determination of chemical oxygen demand.
6. Determination of iron in iron tablets.
7. Simultaneous estimation of chromium (III) and iron (III) by EDTA titration.
8. Simultaneous estimation of calcium (II) and zinc (II) by EDTA titration.
9. Simultaneous estimation of lead (II) and magnesium (II) by EDTA titration.
10. Separation of aminoacids/ dyes/ drugs by TLC.
11. Determination of cation content in hard water by ion exchange chromatography.

**Teaching methodologies:** Practical work, problem solving and group discussion etc.

#### **References books: PCH 2806L (B): Analytical Chemistry (Practicals)**

1. Analytical Chemistry Practice, John H. Kennedy, Saunders College Publishing, Second Edition 1990.
2. Vogel's Textbook of Quantitative Chemical Analysis, 6th Edition, 2002.

**M Sc Organic Chemistry Semester III**  
**Semester III (Organic Chemistry) Overview**

<b>Sub. code</b>	<b>Course</b>	<b>Instruction Hrs/week</b>	<b>Internal Assessment Marks</b>	<b>Max Marks Semester Exams</b>	<b>Duration of Semester Exam (Hrs)</b>	<b>Credit</b>
<b>THEORY</b>						
PCH 3801	Organic Chemistry	4	30	70	3	4
PCH 3802	Organic Chemistry	4	30	70	3	4
PCH 3803	Organic Chemistry	4	30	70	3	4
PCH 3804	Organic Chemistry	4	30	70	3	4

<b>PRACTICALS</b>						
PCH 3805L	Organic Chemistry Lab-I	3	30	70	3	4
	Organic Preparations	3			3	
PCH 3806L	Organic Chemistry Lab-II	3	30	70	3	4
	Organic Estimations	3			3	
<b>Total</b>		<b>28</b>	<b>180</b>	<b>420</b>		<b>24</b>

Note:- Semester -I and Semester-II syllabus is common for all specializations to be selected by the students for final year i.e. Inorganic, Organic, Physical and Analytical. At present St. Xavier's College (Autonomous) offers only Organic Chemistry as a specialization in the final year of M Sc Chemistry.

### **M Sc Organic Chemistry Semester III (Organic Chemistry)**

**CORE Paper: Natural Products and Biomolecules (Theory)**

**Course Code: PCH 3801**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

#### **Course Overview & Course Objectives**

The main objective of the course will be to enhance the understanding and knowledge of Organic Chemistry, for students studying, any branch of chemistry.

By the end of the paper, a student will be able to:

- Understand the important aspects of Natural pigment
- Learn the chemistry of Alkaloids and vitamins
- Understand the important aspects of Steroids and hormones
- Learn the chemistry of Terpenoids and carotenoids.

Thus, the knowledge from the course can help in the following:

- Finally, all students, of all branches whether organic or inorganic will be able to incorporate this knowledge, in their pursuit of research in their different fields.

#### **Course Content**

**Unit-1: Natural pigment**

**(15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Natural pigment]

Natural colouring matter, general classification, method of synthesis, biosynthesis studies of anthocyanins (cyanine) flavones (chryosin) and flavanol (Querecetin)

Porphyrin-structure, spectral properties and synthesis, general and structure determination of Haemoglobin, chlorophyll and Bilirubin.

### **Unit-2: Alkaloids and vitamins (15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Alkaloids and vitamins]

Alkaloids: General biogenetic studies of alkaloids, chemistry of quinine, morphine, reserpine and colchicine

Vitamins : Introduction, Classification, synthesis and biochemical function of vitamin B(Thiamine), Vitamin H and  $\alpha$ -tocopherol (Vitamin E), vitamin C.

### **Unit-3: Steroids and hormones (15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Steroids and hormones]

- Brief account on the chemistry of steroids: structure of cholesterol and ergosterol, Bile acid-Lithiocholic (No synthesis).
- Chemistry of androgens (Androsterone and testosterons), oestrogens-Oestrone and gestrogens- Progesteron, their synthesis and biochemical role

### **Unit-4: Terpenoids and carotenoids (15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Terpenoids and carotenoids]

- Introduction to Terpenes, Classification, nomenclature, general methods of structure determination, chemistry and synthesis, Monoterpenes-Geraniol & terpineol, Sesquiterpenes- farnesol, zingeberine Diterpenoids- abietic acid and gibberellic acid
- Carotenoids : Introduction, classification of carotenoids and B-carotenoids –(Structural elucidation and synthesis of  $\beta$ -carotene – their uses.)

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

### **Reference books: PCH 3801: Natural Products and Biomolecules (Theory)**

- Organic chemistry vol I & II (sixth edition) I.L.Finar

2. Chemistry of vitamins-S.F.Dyke
3. Chemistry of natural products by Bantely, Vol 1-10
4. L.J.Wade Jr. Organic chemistry, Prentice Hall, England cliffs, 1987
5. Chemistry of Natural products vol I & II by O.P.Agrawal
6. Essentials of medicinal chemistry , eds., Korolkovas and Burkhalter, J.H., John wiley & sons
7. Text book of Organic medicinal and pharmaceutical chemistry by Wilson and Gisvold.  
Synthetic drugs by O. D. Tyagi.

### **Semester III (Organic Chemistry)**

#### **CORE Paper: Medicinal Chemistry (Theory)**

**Course Code: PCH 3802**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

#### **Course Overview & Course Objectives**

The main objective of the course will be to enhance the understanding and knowledge of Organic Chemistry, for students studying, any branch of chemistry.

By the end of the paper, a student will be able to:

- a. Understand the important aspects of Antibiotics
- b. Learn the Chemistry of Psychoactive drugs
- c. Understand the important aspects of Antimalarial and Antituberculosis drugs
- d. Learn the Chemistry of Cardiovascular, diuretics and hypoglycemic agents.

Thus, the knowledge from the course can help in the following:

- a. Finally, all students, of all branches whether organic or inorganic will be able to incorporate this knowledge, in their pursuit of research in their different fields.

#### **Course Content**

General classification, structural variations, synthesis and medicinal uses of the following classes of drugs. In addition to the above structure Activity Relationships and Mode of Action should be discussed in classes wherever it is mentioned.

#### **Unit-1: Antibiotics**

**(15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Antibiotics]

- a. The  $\beta$ -lactam antibiotics: Penicillin and cephalosporin  
 Penicillin: Structure determination, Mode of action and Structure activity relationship (SAR), Synthesis of Penicillin V.  
 Cephalosporin: First, second, third and fourth generation of cephalosporin's their SAR, mode of action, Synthesis of Cephalosporin

- b. Non lactum antibiotics: Tetracycline, Chloroamphenicol  
Tetracycline: General characteristics, Mode of action and SAR of tetracyclines  
Chloroamphenicol: Structure, SAR, Mode of action and its synthesis.
- c. Non classifiable antibiotics (only structure and therapeutic uses)  
Bacitracin, vancomycin, nalidixic acid, norfloxacin and ciprofloxacin  
(Only name and structures)

**Unit-2: Psychoactive drugs** (15L) [14 Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Psychoactive drugs]

Introduction, classification, structure activity relationship (SAR), Mode of action of

- a. General and local Anesthetics
- b. Sedative and hypnotics Antipsychotic drugs
- c. Antidepressant
- d. Neuroleptics

and selected synthesis of the following:

Thiopental, amobarbital, diazepam, zaleplon (Sonata), alprazolam, glutethimide, nikethamide, Haloperidol, Aripiprazole, procaine, lidocaine, dibucaine, Fluoxetine and escitalopram

**Unit-3: Antimalarials and Antituberculosis drugs** (15L) [14 Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Antimalarial and Antituberculosis drugs]

- a. Antimalarials: Modern chemotherapy of malaria, 4-amino and 8-amino quinolins, 9-amino acridine. Synthesis of mefloquines, chloroquine, primaquine and daraprim  
Mode of action of antimalarial agents SAR of antimalarial agents.
- b. Anti tuberculosis: Introduction, classification and mode of action, drug resistance tuberculosis. Synthesis of only the following drugs: Isoniazid (INH), Ethionamide, Ethambutol, DDS (Dapsone).

**Unit-4: Cardiovascular, diuretics and hypoglycemic agents** (15L) [14 Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Cardiovascular, diuretics and hypoglycemic agents]

Cardiovascular agents: Introduction, classification, therapeutic drug categories and mode of action of any three category.

Diuretics: Introduction, types of diuretics, mode of action (three categories)

Hypoglycemic agents: Introduction, classification of Type 2 hypoglycemic agents (sensitizers)  
Synthesis of amyl nitrate, diltiazim, atenolol, methyl dopa, tolbutamide, chlorpropamide, glibenclamide, acetazolamide, chlorothiazide, furosemic and ethacrynic acid.

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

**Reference books: PCH 3802: Medicinal Chemistry (Theory)**

1. Burger's medicinal chemistry and drug design (5/e) 1997, vol 1 to 5 edited by Manfred E.Woltt (John wiley and sons Mc. New york)
2. Principles of medicinal chemistry by William A. Foye (ied), lea and febiys (Philadelphia)
3. Principles of medicinal chemistry vol I & II (5/e) F.S.kadam, K.R. Mahadic and K.G.Bohra (Nirali publication)
4. Medicinal chemistry by Ashutosh kar
5. The organic chemistry of drug synthesis vol I, II and III (1980) ed by D. lednicer and L.A. mitscher (Johyn wiley and sons, New york)
6. Wilson and Gisvold text book of organic medicinal and pharmaceutical chemistry (5/e,1982) by Robert Doerge (J.B. lippincoff company, phaladophia/ Toppan co.Ltd, Tokyo)
7. Topics in medicinal chemistry vol I & II by rabinowitz Myerson (interscience 1968)
8. The pharmaceutical basis of therapeutics by Geoman and Gilman (Mcmillan co.)

**Semester III (Organic Chemistry)**

**CORE Paper: Organic Spectroscopy (Theory)**

**Course Code: PCH 3803**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

**Course Overview & Course Objectives**

The main objective of the course will be to enhance the understanding and knowledge of Organic Chemistry, for students studying, any branch of chemistry.

By the end of the paper, a student will be able to:

- a. Understand the various aspects of  $^{13}\text{C}$ -NMR and their applications
- b. Learn the important aspects Mass spectrometry and their applications
- c. Understand the important aspects of NMR and their applications
- d. Learn and practice Structural elucidation based on spectroscopic techniques.

Thus, the knowledge from the course can help in the following:

- a. Finally, all students, of all branches whether organic or inorganic will be able to incorporate this knowledge, in their pursuit of research in their different fields.

**Course Content**



**Unit-1: <sup>13</sup>C-NMR****(15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to <sup>13</sup>C- NMR]

<sup>13</sup>C NMR Spectroscopy: Introduction, Instrumentation and instrumental problems, <sup>13</sup>C- chemical shifts, factors affecting chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants, proton coupled <sup>13</sup>C - spectra, proton decoupled <sup>13</sup>C- spectra. Off- resonance decoupling, DEPT technique.

**Unit-2: Mass Spectroscopy****(15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to and Mass spectrometry]

Mass Spectroscopy: Introduction, Instrumentation, Ionization technique-EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance, mass spectral fragmentation of organic compounds, common functional groups, Detection of molecular ion peak, base peak, metastable ion peak, McLafferty rearrangement, nitrogen rule, high resolution mass spectrometry, examples of mass spectral fragmentation of organic compounds with respect to their structure determination. Hyphenated mass spectroscopy.

**Unit-3: NMR****15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to NMR]

Elementary ideas of NMR integration, chemical shifts, Factors affecting, chemical shifts, coupling (first order, analysis) instrumentation and principles and instrumentation, FT, chemical shifts, spin-spin coupling different spin systems, mechanism of spin coupling, AB, ABX, factors affecting vicinal and geminal couplings, rate processes, long range couplings, spin decoupling, shift reagents, solvent shifts, nuclear overhauser effect. 2D NMR (COSY and HETCOR) applications.

**Unit-4: Structural elucidation****(15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to UV, IR, PMR, CMR and mass spectroscopy]

Structural elucidation of drug molecules based on joint application of UV, IR, PMR, CMR and mass spectroscopy.

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

**Reference books: PCH 3803 : Organic Spectroscopy (Theory)**

1. Spectroscopic methods in organic chemistry, D.H.Williams and Tan Fleming.
2. Spectrometric identification of organic compounds, T.C.Morril R.M.Silverstein and G.Bassler, 6<sup>th</sup> edition, John Wiley and sons
3. Introduction to spectroscopy, D.L.Pavia, G.M.Lampman and G.S.Kriz, 3<sup>rd</sup> edn, Harcourt college publishers.
4. Organic spectroscopy by W.Kemp
5. Organic spectroscopy by P.S.Kalsi

**Paper: PCH 3804: Organic Chemistry (Theory)**

**CORE Paper: Industrial Chemistry (Theory)**

**Course Code: PCH 3804**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

### **Course Overview & Course Objectives**

The main objective of the course will be to enhance the understanding and knowledge of Organic Chemistry, for students studying, any branch of chemistry.

By the end of the paper, a student will be able to:

- a. Understand the important aspects of Unit Processes and Operations.
- b. Learn the various aspects of Green chemistry.
- c. Understand the important aspects of Cosmetics.
- d. Learn the chemistry of Synthetic Dyes and Pigments.

Thus, the knowledge from the course can help in the following:

- a. Finally, all students, of all branches whether organic or inorganic will be able to incorporate this knowledge, in their pursuit of research in their different fields.

### **Course Content**

#### **Unit-1: Unit Processes and Operations**

**(15L) [ 14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental terms related to Unit Processes and Operations]

- a. Nitration, oxidation, sulphonation, reduction, halogenations,
- b. Filtration, extraction, crystallization, drying, distillation and industrial chemicals derived from benzene, naphthalene and anthracene using unit process.

#### **Unit-2: Green chemistry**

**(15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Green chemistry]

Green chemistry -12 principles of green chemistry

Green solvents- aqueous phase reactions, Wurtz reaction, Wittig-Horner reaction, Michael

reaction

Solid phase reactions: halogenation, aldol condensation, grignard reaction.

Ionic liquid as green solvent: hydrogenation, diels-alder reaction, o-alkylation and N-alkylation.

Introduction: green catalysts, green reagents, Microwave Madelung Indole synthesis, Enzymatic

Conversion of sucrose to ethanol.

### Unit-3: Cosmetics

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to cosmetics, Perfumes]

- a. Classification, Raw materials for cosmetics, Manufacturing of various cosmetic products  
Baby Care Product ,Dental Products, Hair Care product
- b. Synthetic Perfumes Definition, classification, synthesis and uses of : ester of cinnamic acid, linalool, phenyl ethyl alcohol, civet one, musk ambrette, alpha and  $\beta$  ionones, alpha and  $\beta$  irones.

### Unit-4: Synthetic Dyes and Pigments

(15L) [14 Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Synthetic Dyes and Pigments]

Introduction, Relation between colour and chemical constitution of dye, hot and cold brand dyes, types of fibers to be dyed, Basic operations in dyeing, Methods of Dyeing of direct, mordant and vat dyes, Classification of dyes according to their applications and chemical constitutions, Fluorescent brightening agents. synthesis of Rosaniline, Tinopal BV, Rhodamine 6G (Red).

Non textile dyes: Leather dyes, Paper dyes, Food colours, Cosmetic dyes, Medicinal dyes.

Pigments: Introduction, Inorganic pigments, application of titanium pigments, organic pigments, chemistry of copper pthalocyanine.

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

### Reference books: PCH 3804: Industrial Chemistry (Theory)

1. Unit processes in organic synthesis by P.H. Groggins
2. Industrial Chemical process by R.N. Shreve
3. Riegels handbook of industrial chemistry ed by James and Kent
4. Dryden's outlines of chemical Technology M. Gopal Rao
5. The chemistry of oils & fats,F.D.Gunstone,Blackwell Pub.
6. Baileys Industrial oils & fats products,Vol 1-5,John Wiley & Sons

7. Essential Oils, Vol 1-7, D. Gunther, R.E. Krigger Pub Comp., New York
8. Cosmetic Science & Technology, Vol 1 & 2, Wiley Interscience, New York
9. Cosmetics, Soaps & Perfumes, W.A. Poucher, Chapman Hall, London & New York
10. Industrial Chemistry by B K Sharma, Sixteenth edition, GOEL publishing house, Meerut.
11. Hand book of Synthetic dyes and Pigments, Vol I, II, III, by K M Shah, second edition, Multi-tech publishing co. Mumbai.

**CORE Paper: Organic Preparations (Practicals)**

**Paper: PCH 3805L:**

**No. of Credits: 04**

**Learning Hours: 60 hrs**

**Course Content**

Preparation of industrially important compounds by following name reactions (mechanism, purification and characterization of the synthesized compounds)

- a. Sandmeyer reaction
- b. Pechmann reaction
- c. Skraup synthesis
- d. Riemeier-Tiemann reaction
- e. Kolbe-smith reaction
- f. Claisen-smith synthesis
- g. Hoffman reaction
- h. Diels-alder reaction
- i. Green –bromination

**Teaching methodologies:** Practical work, problem solving, and group discussion etc.

**References books: PCH 3805L : Organic Preparations (Practicals)**

1. A text book of practical organic chemistry by A. I. Vogel
2. Practical organic Chemistry by Mann and Saunders
3. A handbook of quantitative and qualitative analysis by H. T. Clarke
4. Comprehensive Practical Organic Chemistry : Qualitative Analysis by V K Ahluwalia & S. Dhingra.
5. Comprehensive Practical Organic Chemistry : Preparations and Quantitative Analysis by V K Ahluwalia & R. Aggarwal Universities Press.
6. An Advance Course in practical Chemistry, by A K. Nad, B. Mahapatra and A. Ghoshal.

Sub. code	Course	Instructi on Hrs/wee k	Internal Assesse ment Marks	Max Marks Semeste r Exams	Duratio n of Semeste r Exam (Hrs)	Credi t
<b>THEORY</b>						
PCH 4801	Organic Chemistry	4	30	70	3	4
PCH 4802	Organic Chemistry	4	30	70	3	4
PCH 4803	Organic Chemistry	4	30	70	3	4
PCH 4804	Organic Chemistry	4	30	70	3	4
<b>PRACTIC ALS</b>						
PCH 4805L	Organic Chemistry Lab-I	3	30	70	3	4
	Industrial training	3			3	
PCH 4806L	Organic Chemistry Lab-II	3	30	70	3	4
	Organic Preparations and Estimation	3			3	
<b>Total</b>		<b>28</b>	<b>180</b>	<b>420</b>		<b>24</b>

**CORE Paper: Organic Estimations (Practicals)**

**Paper: PCH 3806L:**

**No. of Credits: 04**

**Learning Hours: 60 hrs**

**Course Content**

**1. Estimations and Extractions**

- a. Drug assay (estimation of sulpha drug)
- b. Non-aqueous titration (Nicotine estimation in  $\text{HClO}_4$ )
- c. Nitrite value
- d. Extraction of Casein from Milk

**Teaching methodologies:** Practical work, problem solving, and group discussion etc.

**References books: PCH 3806L : Organic Estimation (Practicals)**

1. Quantitative analysis by Arther I.Vogel
2. Quantitative analysis by V.K.Ahluwalia
3. Quantitative analysis by Mann and sanders

**Semester VI**

Note:- Semester -I and Semester-II syllabus is common for all specializations to be selected by the students for final year i.e. Inorganic, Organic, Physical and Analytical. At present St. Xavier's College (Autonomous) offers only Organic Chemistry as a specialization in the final year of M Sc Chemistry.

**M Sc Semester IV (Organic Chemistry)**

**CORE Paper: Advanced Organic Chemistry (Theory)**

**Course Code: PCH 4801**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

**Course Overview & Course Objectives**

The main objective of the course will be to enhance the understanding and knowledge of Organic Chemistry, for students studying, any branch of chemistry.

By the end of the paper, a student will be able to:

- a. Understand the important aspects of Pericyclic reactions
- b. Learn various aspects of Conformational analysis
- c. Understand the important aspects of Aliphatic Electrophilic substitutions
- d. Learn the chemistry of Modern Synthetic Methods

Thus, the knowledge from the course can help in the following:

- a. Finally, all students, of all branches whether organic or inorganic will be able to incorporate this knowledge, in their pursuit of research in their different fields.

**Course Content**

**Unit-1: Pericyclic reactions**

**(15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Pericyclic reactions]

Introduction, classification of pericyclic reactions, stereochemistry, molecular orbital symmetry,

frontier orbitals of ethelene, 1,3 –butadiene, 1,3,5-hexatriene and allyl system, F.M.O. and PMO approach to cycloaddition and electrocyclic reactions: Generalization of wood-ward Hoffmann rule, sigmatropic rearrangement-suprafacial and antrafacial shifts of H.Stereoselectivity in sigmatropic rearrangement, enantioselectivity in pericyclic reactions.

**Unit-2: Conformational analysis (15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Conformational analysis]

Confirmation at cyclic systems: Confirmation of cyclohexane, mono and disubstituted cyclohexane, heterocyclic compounds, five and six membered heterocycles, stereoelectronic effects, fused bicyclic sptem, decalin, dodecalin, polyclin system, perhydrophenanthrene, bridged systems-conformation of sugars, steric strains due to unavoidable crowding, stereochemistry of the compounds containing nitrogen, sulphur and phosphorous.

**Unit-3: Aliphatic Electrophilic substitutions (15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Aliphatic Electrophilic substitutions]

Aliphatic Electrophilic substitutions: SE1 SE2 and SEi Bimolecular mechanisms, electrophilic substitution accompanied by double bond shifts, migration of double bonds, Hydrogen, Halogen, nitrogen, carbon sulphur and metal as electrophiles and their reactions (selective reactions only). Metal and Halogen as leaving group.

**Unit -4: Modern Synthetic Methods (15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Modern Synthetic Methods]

Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Ugi reaction, Noyori reaction. Brook rearrangement. Tebbe olefination.

Introduction to chemistry of multicomponent reactions and Click reactions. Domino/cascade reactions: Introduction with one example.

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

**Reference books: PCH 4801 : Advanced Organic Chemistry (Theory)**

1. Advanced organic chemistry - Reaction mechanism and structure, Jerry March, John Wiley publication.
2. Structure and mechanism in organic chemistry, C. K. Ingold, Cornell University Press.
3. Advance organic chemistry by Francis A. Carey
4. Named organic reactions by Laslo Kurti
5. Advanced organic chemistry, Part I & II F. A. Carey and R. J. Sundberg, Plenum.

#### **Semester IV (Organic Chemistry)**

#### **CORE Paper: Advanced Organic Synthesis (Theory)**

**Course Code: PCH 4802**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

#### **Course Overview & Course Objectives**

The main objective of the course will be to enhance the understanding and knowledge of Organic Chemistry, for students studying, any branch of chemistry.

By the end of the paper, a student will be able to:

- a. Understand the important aspects of Protection of groups
- b. Learn the various aspects of Disconnection approach
- c. Understand the chemistry of One group C-C disconnections
- d. Learn the chemistry of Ring synthesis of heterocyclic compounds

Thus, the knowledge from the course can help in the following:

- a. Finally, all students, of all branches whether organic or inorganic will be able to incorporate this knowledge, in their pursuit of research in their different fields.

#### **Course Content**

##### **Unit-1: Protection of groups**

**(15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Protection of groups]

Principle of protection of hydroxyl, amino, carbonyl, carboxylic acid with different reagents and their de protection, synthetic equivalent groups, synthetic analysis and planning, control of stereochemistry.

##### **Unit-2: Disconnection approach**

**(15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Disconnection approach]

An introduction to synthesis, and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis one group C-X and two group C-X disconnections, chemo-selectivity, reversal and polarity.



**Unit-3: One group C-C disconnections** (15L) [14 Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to : One group C-C disconnections]

Alcohols and carbonyl compounds, region-selectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

**Unit-4: Ring synthesis of heterocyclic compounds** (15L) [14 Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to ring synthesis]

Saturated heterocycles, synthesis of 3, 4, 5, and 6-membered rings, aromatic heterocycles in organic synthesis.

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

**Reference books: PCH 4802 : Advanced Organic Synthesis (Theory)**

1. Organic synthesis : the disconnection approach by Stuart Warren (Wiley student edition)
2. Organic chemistry- Clayden, Greeves, Warren and Wothers, (Oxford Press)
3. Structure and mechanism in organic chemistry, C. K. Ingold, Cornell University Press.
4. Advanced organic chemistry, Part I & II F. A. Carey and R. J. Sundberg, Plenum.

**Semester VI**

**CORE Paper: Bioorganic Chemistry (Theory)**

**Course Code: PCH 4803**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

**Course Overview & Course Objectives**

The main objective of the course will be to enhance the understanding and knowledge of Organic Chemistry, for students studying, any branch of chemistry.

By the end of the paper, a student will be able to:

- a. Understand the important and fundamental aspects of Biochemistry
- b. Learn the chemistry of Metabolism and Metabolic Reaction
- c. Understand the important aspects of Nucleic Acids
- d. Learn the chemistry of selected topics in Carbohydrate and Vitamin Chemistry

Thus, the knowledge from the course can help in the following:

- a. Finally, all students, of all branches whether organic or inorganic will be able to incorporate

this knowledge, in their pursuit of research in their different fields.

## **Course Content**

### **Unit-1: Fundamentals of Biochemistry**

**(15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Fundamentals of Biochemistry]

Introduction of Biochemistry, Amino acids: peptides, primary, secondary, tertiary, and quaternary structure of proteins. Nucleic acids: Base pairing, double helices, DNA replication, transcription and translation, Enzymatic hydrolysis of proteins to peptides; Amino acid sequencing; amino acid metabolism (biosynthesis and degradation).

### **Unit-2: Metabolism and Metabolic Reaction**

**(15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Metabolism and Metabolic Reaction]

Overview and important relationships between-glycolysis, Bioenergetics And Bio energetic principles, oxidative phosphorylation process, ATP synthetize, photophosphorylation.

1. **Fatty acid metabolism:** Biological importance of fatty acids and lipids, even chain and odd chain fatty acids, saturated and unsaturated fats, ketone bodies, fatty acid metabolism, calorific value of foods, biological membranes, properties and function of lipid bilayers and liposomes.
2. **Protein-related transformations:** urea cycle, uric acid and ammonia formation.

### **Unit-3: Nucleic Acids**

**(15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Nucleic Acids]

Chemical and enzymatic hydrolysis of nucleic acids; Structure and function of mRNA, tRNA, rRNA; Polymorphic nature of DNA, B-and Z-DNA, multi-stranded DNA; DNA sequence determination by chemical and enzymatic methods, Genetic code–origin, salient features, Gene expression transcription and translation; Gene mutation and carcinogenesis

### **Unit-4: Selected topics in Carbohydrate and Vitamin Chemistry**

**(15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to selected topics in Carbohydrates and Vitamins]

Carbohydrates: classification and stereochemistry, biologically important hexose derivatives, nomenclature of disaccharides, structure and role of some homo and hetero polysaccharides, polysaccharides: starch and cellulose, glycosides: salicin, indican and amygdalin, glucoconjugates : proteoglycans, glycoproteins and glycolipids.

Vitamins : Synthesis and biochemical function of vitamin A, vitamin D and vitamin K.

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

**Reference books: PCH 4803: Bioorganic Chemistry (Theory)**

1. Albert L. Lehninger, David L. Nelson, Michael M. Cox., Principles of Biochemistry, CBS Publishers and Distributors, 1993.
2. Lubert Stryer, Biochemistry, W. H. Freeman and Company, 4th edition, 1995.
3. Christopher K. Mathews and K. E. Von Holder, Biochemistry, Benjamin/Cummings, 1990.
4. Eric E. Conn, Paul K. Stumpf, George Brening and Roy H. Doi, Outlines of Biochemistry, 5th edition, John Wiley and Sons, 1987.
5. Organic Chemistry by F. A. Carey and R. J. Sundberg, (Eds) 3rd Edition, Part B. Plenum/Rosetta, 1990.
6. Fleming, Selected Organic Synthesis, John Wiley and sons, 1982.
7. Atta-ur-Rehman, Studies in Natural Products Chemistry, Vol.1 and 2, Elsevier, 1988.
8. T. Lindberg, Strategies and Tactics in Organic Synthesis, Academic Press, 1984.
9. E. J. Corey and X-M. Cheng, Logic of Chemical Synthesis, John Wiley, 1989.
10. H. Pape and J. H. Rehm, (eds): Biotechnology, A Comprehensive Treatise, Vol. 1-8, VCH, 198
11. Principles of biochemistry – Donald J. Voet, Judith G. Voet, Charlotte w. Pratt (John Wiley and sons)
12. Lehninger principles of biochemistry- David L. Nelson and Michael M. (Palgrave Macmillan / w.h. freeman company new york)
13. Biochemistry – U. Satyanarayana Baro and allied P. Ltd., Kolkata

**Semester VI**

**CORE Paper: Selected topics in Medicinal Chemistry (Theory)**

**Course Code: PCH 4804**

**No. of Credits: 04**

**Learning Hours: 60 hrs (70 Marks)**

**Course Overview & Course Objectives**

The main objective of the course will be to enhance the understanding and knowledge of Organic Chemistry, for students studying, any branch of chemistry.

By the end of the paper, a student will be able to:

- a. Understand the important aspects of Drug design
- b. Learn the chemistry of Pharmacokinetic and pharmacodynamics

- c. Understand the important aspects of Quality control and computer applications in pharma industries
- d. Learn the chemistry of selected topics in Nano science and Medicinal chemistry.

Thus, the knowledge from the course can help in the following:

- a. Finally, all students, of all branches whether organic or inorganic will be able to incorporate this knowledge, in their pursuit of research in their different fields.

## Course Content

### **Unit-1: Drug design** (15L) [14 Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Drug design ]

Introduction, naming of organic medicinal compounds, literature of medicinal chemistry, development of new drugs, procedure followed in drug design, concept of lead compound and lead modification, pro drugs, soft drugs, phase I, II and III clinical trials, structure activity relationship, theories of drug activity : occupational theory, rate theory, induced fit theory, quantitative structure activity relationship, history and development of QSAR. Concept of drug receptors, elementary treatment of drug receptor interactions, physio chemical parameters lipophilicity, partition coefficient, electronic ionization constant, concept of 3-D QSAR.

### **Unit-2: Pharmacokinetic and pharmacodynamics** (15L) [14 Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Pharmacokinetic and pharmacodynamics]

Pharmacokinetics : introduction to drug absorption, distribution, metabolism, elimination. important pharmacokinetic parameters in defining drug deposition and in therapeutics, uses of pharmaceutics in drug development process

Pharmacodynamics: Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, drug metabolism, biotransformation, significance of drug metabolism in medicinal chemistry.

### **Unit-3: Quality control and computer applications in pharm industries** (15L) [14 Marks]

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Quality control and computer applications in pharm industries]

1. Dosage forms, Quality control and application of computers in chemistry  
Dosage forms, types of dosages, different routes of administration, quality control of drugs pharmacopias, modern methods of pharmaceutical analysis.
2. Computer in chemistry  
Use of computer in chemistry and industry  
Important websites for data search chemistry  
Information about online journals for chemistry

#### **Unit-4: Nano science and Medicinal chemistry**

**(15L) [14 Marks]**

[Prerequisites or topics for Self Study: Basic terms and fundamental aspects related to Nano science and Medicinal chemistry]

Overview, Medicinal use of nanomaterials-Drug delivery

Protein and peptide delivery –cancer, surgery, visualization, nanoparticle targeting

Medical application of molecular nanotechnology-nanorobots, cell repair machines, nanonephrology.

**Teaching methodologies:** Apart from the conventional black board teaching, other modes of teaching that will be adopted are power points, problem solving, and group discussion. Assignments will be designed such that students inculcate the habit of reading reference books and science journals. The use of smart boards for teaching will also be promoted to enable more interaction based teaching.

#### **Reference books: PCH 4804 : Selected topics in Medicinal Chemistry (Theory)**

1. Burger's Medicinal Chemistry and Drug Discovery (5/e), 1997, Vol. 1, 2, 3, 4,5, Edited by Manfred E. Wolff (John Wiley & Sons, inc., New York).
2. Wilson and Gisvold's Text-book of Organic Medicinal and Pharmaceutical Chemistry (5/e, 1982) by Robert F. Doerge (J. B. Lippincott Company, Philadelphia/Toppan Co. Ltd., Tokyo).
3. Principles of Medicinal Chemistry, Vol. I & II (5/e), by S. S. Kadam, K. R. Mahadik, K. G. Bothra (Nirali Prakashan).
4. QSAR: quantitative structure-activity relationships in drug design by Jean-Luc Fauchère. ISBN:084515141X, 9780845151419.
5. QSAR : Hansch analysis and related approaches By Hugo Kubinyi

#### **Semester VI**

#### **CORE Paper: Industrial training (Practicals)**

**Course Code: PCH 4805L**

**No. of Credits: 04**

**Learning Hours: 60 hrs**

#### **Course Content**

Industrial training for 21 days, report preparation, submission and presentation / viva

**Learning methodologies:** Training, Practical work, problem solving, and group discussion etc.

#### **References: PCH 4805L: Industrial training (Practicals)**

1. Industrial Chemistry, by B. K. Sharma , GOEL Publishing House, Meerut.

2. Elementary Practical Organic Chemistry, Part I, II and III by Arthur I. Vogel.
3. Practical organic Chemistry, by F. G. Mann and B. C. Saunders, 4<sup>th</sup> Edition.
4. Instrumental Analysis, by William Kemp, 3<sup>rd</sup> Edition.
5. The reference material provide by the industries and the books related to the area of the training.

### **Semester IV (Organic Chemistry)**

#### **CORE Paper: Organic Preparations and Estimation (Practicals)**

**Course Code: PCH 4806L**

**No. of Credits: 04**

**Learning Hours: 60 hrs**

#### **Course Content**

##### **1. Organic Preparations**

1. Preparation of cinnamic acid form benzaldehyde.
2. Preparation of benzophenone oxime from benzophenone
3. Preparation of anthraquinone form anthracene
4. Preparation of 4-phenyl-6-methyl-5-carbethoxy-2-pyrimidone from urea, benzaldehyde, EAA (Ethyl Aceto Acetate)
5. Preparation of 2-phenylindole from acetophenone and phenylhydrazine.
6. Preparation of 2-methylbenzimidazole from *o*-phenylene diamine
7. Preparation of 1, 1-bis-2-naphthol from 2-Naphthol.

##### **2. Organic Estimation**

- a. Estimation of Aspirine
- b. Estimation of Isoniazid (INH)
- c. Estimation of Ibuprofen

**Learning methodologies:** Training, practical work, problem solving, group discussion etc.;

#### **References books: PCH 4806L: Organic Preparations and Estimation (Practicals)**

1. A text book of practical organic chemistry by A. I. Vogel
2. Practical organic Chemistry – Mann and Saunders
3. A handbook of quantitative and qualitative analysis by H. T. Clarke
4. Comprehensive Practical Organic Chemistry : Qualitative Analysis V K Ahluwalia and S. Dhingra.
5. Comprehensive Practical Organic Chemistry : Preparations and Quantitative Analysis V K Ahluwalia and R. Aggarwal Universities Press.
6. An Advance Course in practical Chemistry, A K. Nad, B. Mahapatra and A. Ghoshal.
7. Quantitative analysis by Arther I.Vogel

8. Quantitative analysis by V.K.Ahluwalia
9. Quantitative analysis by Mann and sanders