## **University of Pune**

## Two Year M. Sc. Degree Course in Chemistry

## M. Sc. Chemistry

(Credit and Semester based Syllabus to be implemented from Academic Year 2015-16)

1) Title of the Course: M.Sc. Chemistry

#### 2) Preamble of the Syllabus:

Master of Science (M.Sc.) in Chemistry is a post graduation course of University of Pune. The credit system to be implemented through this curriculum, would allow students to develop a strong footing in the fundamentals and specialize in the disciplines of his/her liking and abilities.

The students pursuing this course would have to develop in depth understanding of various aspects of the subject. The conceptual understanding, development of experimental skills, designing and implementation of novel synthetic methods, developing the aptitude for academic and professional skills, acquiring basic concepts for structural elucidation with hyphenated techniques, understanding the fundamental biological processes and rationale towards computer assisted drug designing are among such important aspects.

#### 3) Introduction:

#### **Salient Features of the Credit System:**

- 1. Master's degree course in Chemistry would be of 100 credits, where one credit course of theory will be of one clock hour per week running for 15 weeks and one credit for practical course will consist of 15 of laboratory exercise including the revision and setting up the practical. Thus, each credit will be equivalent to 15 hours.
- 2. Student will have to take admission in Chemistry Department and complete 75 credits incorporated in the syllabus structure of Chemistry. The remaining 25 credits shall be chosen from courses offered by the Chemistry Department or other Departments of the University/College with credit system structure.
- 3. Except practical credits wherever applicable, students may be allowed to complete less courses per semester on the condition they complete the degree in maximum of four years. This facility will be available subject to the availability of concerned courses in a given semester and with a maximum variation of 25 credits (in case of fresh credits) per semester.
- 4. Every student shall complete 100 credits in a minimum of four semesters. All Semesters will have average 25 credits each.
- 5. The student will be declared as failed if s/he does not pass in all credits within a total period of four years. After that such students will have to seek fresh admission as per admission rules prevailing at that time.
- 6. Academic calendar showing dates of commencement and end of teaching, internal assessment tests and term end examination will be prepared and duly notified before commencement of each semester every year.
- 7. Project course should not be greater than 5% of the total credits of the degree course. Project course is equivalent to 4 credits.

#### **Instructions for the Students**

The students seeking admission to M.Sc. Chemistry course is hereby informed that they are supposed to adhere to the following rules:

- 1. A minimum of 75 % attendance for lectures / practical is the pre-requisite for grant of term.
- 2. There shall be tutorial / practical / surprise test / home assignment / referencing of research papers / seminar / industrial visits / training course as a part of internal assessment in each semester. The students are supposed to attend all the tests. The students should note that retest will not be given to the student absent for the test/s.
- 3. The students opting for dissertation course shall follow the rules framed for the same.
- 4. Industrial / Institute Visit and or Industrial Workshops / Laboratory Workshops / Training Programme is a compulsory component of the syllabus. The students are supposed to attend all the Industrial Workshops / Laboratory Workshops / Training Programme organized by the department. The students shall attend these programs at their own cost.

#### 4) Eligibility:

The candidate should have a B.Sc. degree with Chemistry as principal subject <u>OR</u> B.Sc. (General) degree with Chemistry (Electronics) as one of the subsidiary subjects.

Admission: Admissions will be given as per the selection procedure / policies adopted by the respective college, in accordance with conditions laid down by the University of Pune. Reservation and relaxation will be as per the government rules.

#### 5) Examination

#### [A] Pattern of Examination

**Evaluation of Students:** 

- 1) The In-semester and End-Semester examinations will be of 50 marks each.
- 2) Student has to obtain 40% marks in the combined examination of In-Semester and End-Semester assessment with minimum passing of 30% passing in both assessments separately.
- 3) A student cannot register for third semester if s/he fails to complete the 50% credits of the total expected within two semesters.
- 4) Internal marks will not change. Student cannot repeat internal assessment. If student misses internal assessment examination, s/he will have second chance with the permission of the concerned teacher. But it will not be right of the student. It will be the discretion of the concerned teacher and internal departmental assessment committee. In case s/he wants to repeat Internal, s/he can do so only by registering for the said courses during 5<sup>th</sup>/6<sup>th</sup> semester whichever is applicable.
- 5) There shall be revaluation of answer script of end semester examination, but not of internal assessment papers.
- 6) Internal assessment answer scripts may be shown to the concerned student but not end semester answer script.

- i. In-semester Examination: Internal assessment for each course would be continuous and dates for each tutorials/practical tests will be pre-notified in the time table for teaching or placed separately as a part of time table. Department / College Internal Assessment Committee will coordinate this activity
  - a) Theory Courses: Conducting written tests should not be encouraged. More focus should be on non-written tests. Students should be encouraged to conduct various academic activities. A teacher must select a variety of the procedures for internal assessment suggested as follows.
    - a) Mid-term test
    - b) On-line test
    - c) Computer based examination
    - d) Open book test (concerned teacher will decide the allowed books)
    - e) Tutorial
    - f) Surprise test
    - g) Oral
    - h) Assignments
    - i) Review of research paper
    - j) Seminar presentation
    - k) Journal/Lecture/Library notes

Student has to preserve the documentation of the internal assessment except midterm test answer script. It is the responsibility of the student to preserve the documents.

- **b) Practical Courses**: It is a continuous evaluation process. Practical courses will be evaluated on the basis of the following
  - 1. Performance assessment of each experiment on the basis of attendance, punctuality, journal completion, practical skills, results, oral and analysis.
  - 2. Test on practical may be conducted before the end-semester examination.
  - 3. Assessment of each experiment shall be done for each practical weekly.
  - 4. Assessment of the Activity will be based on any one of the following per practical course.
    - i. Experimental and analytical skills
    - ii. Synthesis of compounds
    - iii. Evaluation of physical constants, purity of compounds
    - iv. Fundamental understanding of instrumental techniques
    - v. Recording and analysis of spectral data
    - vi. Economic utilization of chemicals
    - vii. Basic understanding of the experiment

The student strength of practical batch should be eight. Note that one practical session of 4 hour duration of one practical batch.

**Project Course:** Project will be evaluated by In-Charge of project batch in concern with project guide. Assessment will be done weekly in the respective batch. Evaluation will be on the basis of weekly progress of project work, progress report, referencing, oral, results and documentation.

**ii. End-Semester Examination**: End-Semester examination for 50 marks per course would be held about two weeks after completion of teaching for the semester. Paper setting and assessment for a particular course would be the responsibility of the course In-charge, and these activities would be coordinated by the Department Examination Committee. The Department Examination committee would undertake preparation of the result-sheets for the student

#### [B] Standard of Passing

Student has to obtain 40% marks in the combined examination of In-Semester and End-Semester assessment with minimum passing of 30% passing in both assessments separately.

#### [C] ATKT Rules

A student cannot register for third semester if s/he fails to complete the 50% credits of the total credits expected to be ordinarily completed within two semesters.

#### [D] Award of Class

Grades will be awarded from grade point average (GPA) of the credits.

#### **GPA Rules:**

- 1. The formula for GPA will be based on Weighted Average. The final GPA will not be printed unless a student passes courses equivalent to minimum 100 credit hours (Science). Total credits hours means the sum of credit hours of the courses which a student has passed.
- 2. A seven point grade system [guided by the Government of Maharashtra Resolution No. NGO 1298 / [4619] / UNI 4 dt. December 11, 1999 and University regulations] will be followed. The corresponding grade table is attached herewith.
- 3. If the GPA is higher than the indicated upper limit in the third decimal digit then the student be awarded higher final grade (e.g. a student getting GPA of 4.492 may be awarded 'A')
- 4. For Semester I, II, III examinations, only the grade points will be awarded for each subject. Final GPA along with final grade will be awarded only at the end of IV semester. There is also a provision for verification and revaluation. In case of verification, the existing rules will be applicable. The revaluation result will be adopted if there is a change of at least 10% marks and in the grade of the course.
- 5. After the declaration of result, for the improvement of Grade, the student can reappear for the examination of 30 credits worth theory courses.
- 6. Grade improvement programme will be implemented at the end of the academic year. A student can opt for grade improvement programme only after the declaration of final semester examination i.e. at the end of next academic year after passing M.Sc. (Chemistry) examination and within two years of completion of M.Sc. (Chemistry). A student can appear for grade improvement programme only once.

Grade and Grade Point Average					
Marks	Marks Obtained Grade				
100 – 75	'O' Outstanding	06			
74 – 65	'A' Very Good	05			
64 – 55	<b>'B'</b> Good	04			
54 – 50	'C' Average	03			
49 – 45	'D' Satisfactory	02			
44 – 40	<b>E'</b> Pass	01			
39 and less	<b>'F'</b> Fail	00			

Final Grade Points				
Grade Points	Final Grade			
5.00 - 6.00	0			
4.50 – 4.99	A			
3.50 – 4.49	В			
2.50 – 3.49	С			
1.50 – 2.49	D			
0.50 – 1.49	E			
0.00 - 0.49	F			

Common Formula for Grade Point Average (GPA):

$$GPA = \frac{Total \ of \ Grade \ Points \ earned \ \times \ Credit \ hours \ for \ each \ course}{Total \ Credit \ hours}$$

B Grade is equivalent to at least 55% of the marks

[E] External Students: There shall be no external students.

#### [F] Setting of Question Paper / Pattern of Question Paper

For core (compulsory) theory courses, end semester question papers set by the University of Pune and centralized assessment for theory papers done as per the University instructions. Questions should be designed to test the conceptual knowledge and understanding of the basic concepts of the subject.

Theory examination will be of 2 hours duration for each theory course of 5 credits. There will be **two sections** for each paper. Each section will be of **25 marks** and the pattern of question paper shall be:

Question 1 (10 Marks)	5 compulsory sub-questions, each of 2 marks; answerable in 2-3 lines
Question 2 (10 Marks)	2 out of 4 – short answer type questions of 5 marks each; answerable in 8 – 10 lines
Question 3 (5 Marks)	1 out of 2 – numerical problem type question; note, spectral analysis, functioning of instrumental technique with components

#### [G] Verification / Revaluation

There is also a provision for verification and revaluation. In case of verification, the existing rules will be applicable. The revaluation result will be adopted if there is a change of at least 10% marks and in the grade of the course. There shall be revaluation of answer script of end semester examination, but not of internal assessment papers.

#### 6) Structure of Course

Basic structure/pattern (Framework) of the proposed postgraduate syllabus for the two year integrated course leading to M.Sc. (Chemistry) in the colleges affiliated to Pune University.

#### a) Compulsory Papers

Theory: CHP-110, CHP-210, CHI-130, CHI-230, CHO-150, CHO-250,

CHA-290

Practical: CHP-107, CHI-147, CHO-247

M. Sc. Chemistry - Course structure & Credits Distribution

Semester	Course Code	Course Title	No. of Units	No. of credits
	CHP-110	Fundamentals of Physical Chemistry-I	04	04
	CHI-130	Molecular Symmetry & Chemistry of p- block elements	04	04
	CHO-150	Basic organic chemistry	04	04
Sem-I	CHA-190	Safety in Chemical Laboratory and Good Laboratory Practices	04	04
	CHP-107	Practical Course (Physical Chemistry)	24 Practical Sessions	06
	CHI-147	Practical Course (Inorganic Chemistry)	24 Practical Sessions	06
	CHP-210	Fundamentals of Physical Chemistry-II	04	04
Sem-II	CHI-230	Coordination and Bioinorganic Chemistry	04	04
	CHO-250	Synthetic organic chemistry and spectroscopy	04	04
	CHA-290	General Chemistry	04	04
	СНО-247	Practical Course (Organic Chemistry)	24 Practical Sessions	06

- **CHA-290** is not Departmental but the University course and the exam for 50 marks will be conducted by the University.
- 2. Part F: Pericyclic, Photochemistry and Free Radical should be treated as Part G
- 3. There are 7 optional courses of each **2 credits except part B which is of 4 credits** for CHA-290 course. These are:
  - Part A: Modern Separation Methods and Hyphenated techniques.
  - Part B: Basic Biochemistry (Compulsory for Drug and Medicinal Chemistry Specialization).
  - Part C: Concept of Analytical Chemistry.
  - **Part D**: Industrial Methods of Analysis.
  - **Part E**: Organometallic and Inorganic Reaction Mechanism (Recommended for Specializations other than Inorganic Chemistry).
  - **Part F**: Mathematics for Chemists (Recommended for Specializations other than Physical Chemistry).
  - **Part G**: Pericyclic, Photochemistry and Free Radical (Recommended for Specializations other than Organic Chemistry).

While choosing this course, kindly take note of following choices.

Sr. No.	Specialization	Available Optional Subjects	Choice
1	Physical Chemistry	A, C, D, E and G	Any two from these options
2	Inorganic Chemistry	A, C, D, F and G	Any two from these options
3	Organic Chemistry	A, C, D, E and F	y two from these options
4	Analytical Chemistry	A compulsory and any one from C, D, E, F and G	any one from remaining
5	Drug Chemistry	B compulsory	B compulsory
6	Polymer Chemistry	A, C, D, E, F and G	y two from these options
7	Medicinal Chemistry	<b>B</b> compulsory and any one from A, C, D, E, F and G	B + any one from remaining

#### b) Question Papers and papers etc.:

Theory

In-Semester Examination: 50 Marks End-Semester Examination: 50 Marks

**Practical** 

In-Semester Examination: 50 Marks End-Semester Examination: 50 Marks

c) Medium of Instructions: English.

#### 7) Equivalence of Previous Syllabus:

New Course ( 5 credit pattern;	New Course ( 4 Credit pattern; 2014 - 15 Pattern)			
<b>20013-14 Pattern</b> )				
CH-110	CHP-110			
CH-130	CHI-130			
CH-150	CHO-150			
-	CHA-190			
CH-107	CHP-107			
CH-127	CHI-127			
CH-210	CHP-210			
CH-230	CHI-230			
CH-250	CHO-250			
CH-290	CHA-290			
CH-247	CHO-247			

#### 8) University Terms:

Dates for commencement and conclusion for the first and second terms will be declared by the University authorities. Terms can be kept by only for duly admitted students. The term shall be granted only on minimum 75 percent attendance at theory and practical course and satisfactory performance during the term.

#### 9) Qualification of Teacher:

- i. M.Sc. (Chemistry) degree with NET/SET qualification.
- ii. Recognition of Pune University as a post graduate teacher, by apers.
- iii. Other criteria as per the guidelines of UGC and University of Pune.

## M. Sc. Chemistry Part-I

## **Physical Chemistry**

#### Semester - I

#### CHP-110: Fundamentals of Physical Chemistry-I

(4 Credits)

**SECTION-I** 

(2 Credits, 24 L, 6 T)

## **Thermodynamics**

- Recapitulation:- Heat, work & Conservation of energy The basic concepts, the first law, infinitesimal changes, mechanical work, work of compression & expansion, free expansion, expansion against constant pressure, reversible expansion. Heat:- heat capacity, enthalpy. State functions & differentials State functions, exact & inexact differential, changes in internal energy, temperature dependence of the internal energy, temperature dependence of the enthalpy. Work of adiabatic expansion Irreversible adiabatic expansion, reversible adiabatic expansion.
- 2. The second law of Thermodynamics: Measuring the dispersal the entropy. The second law, the definition of entropy, the entropy changes in the system, natural events. Entropy changes in the universe The enthalpy change when a system is heated. Entropy changes in surroundings. The entropy of phase transition. The entropy of irreversible changes. Concentrating on the system The Helmholtz & Gibbs function, some remarks on the Helmholtz function. Maximum work, some remarks on Gibbs function. Evaluating the entropy & Gibbs function. The third law of Thermodynamics, Third law entropies standard molar Gibbs function.
- 3. Combining First & Second law One way of developing the fundamental equations properties of Gibbs function. The temperature dependence of the Gibbs functions. The pressure dependence of the Gibbs functions. The chemical potential of a perfect gas. The open system & changes of composition.
  (03 L)

- 4. Changes of State: Physical Transformation of pure materials. The stabilities of phases, Phase equilibrium & phase diagrams. The solid liquid boundary. The liquid vapor boundary. The solid-liquid-vapor boundary. (03 L)
- 5 Changes of State: Physical transformation of simple mixtures, partial molar quantities Partial molar volume, Partial molar Gibbs function. The thermodynamics of mixing the Gibbs function of mixing after thermodynamics mixing functions. The chemical potential of liquid-liquid mixture. Colligative properties The common features, the elevation of boiling point. The depression of freezing point, solubility, osmosis. Mixtures of volatile liquid-vapor pressure diagram. (04 L)

Historical development of quantum theory, failure of classical mechanics, black body radiation, photo electric effect, specific heats of solids, Atomic spectra, wave particle duality, uncertainty principles, Schrodinger equation, free particle, particle in one dimensional box, hydrogen like atoms (No derivation), atomic orbital's.

#### **SECTION-II**

(2 Credits, 24 L, 6 T)

## Chemical kinetics and reaction dynamics

- Recapitulation: The rates of reaction, reaction rate, rate laws & rate constants, the
  determination of the rate law, first order, second order reactions, half lives, fractional order
  reactions.
- Accounting for rate laws, simple reactions, the temperature dependence of reaction rates, reactions approaching equilibrium, consecutive reactions, the steady state approximations, pre equilibria, unimolecular reactions. (05 L)
- 3. The kinetics of complex reactions: chain reaction- explosion, photochemical reactions-quantum efficiency, fast reactions-flash photolysis, flow techniques, relaxation methods.

(02 L)

- 4. Molecular reaction dynamics- collision theory-the basic calculations, the steric requirements, Diffusion control reactions- classes of reactions, diffusion and reactions, the details of diffusion, Activated complex theory- the reaction coordinate and the transition state, the formation and decay of the activated complex, how to use the Eyring equation, thermodynamics aspects, reactions between ions. (05 L)
- 5. Enzyme catalysts: Michaelis-Menten mechanism, limiting rate, Lineweaver Burk and Eadie plots enzyme inhibition, competitive and non-competitive inhibition. (04 L)
- 6. Molecular Thermodynamics: Molecular energy levels, Boltzmann distribution law, partition functions and ensembles, translational, rotational and vibrational partition functions of diatomic molecules, Obtaining energy, heat capacity, entropy free energy, equilibrium constants from partition functions, equipartition of energy, Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein statistics. (06 L)

#### References

- 1. Physical Chemistry- P.W.Atkin and De Paule 8th edition (2010)
- 2. Physical Chemistry-T. Engel and P. Reid, Pearson Education (2006)
- 3. Physical Chemistry and molecular approach- D. Mcquarie and J. Simon (University Science) (2000)
- 4. Physical Chemistry for Bilogical Sciences by Raymond Change (Universal books ) (2000)
- 5. Physical Chemistry Marron and Prouton
- 6. Physical Chemistry- G.M. Barrow, Tata McGrow Hill 1988
- 7. Quantum Chemistry- I. Levine 5<sup>th</sup> edition, Prentice Hall, 1999.

## **Inorganic Chemistry**

## Semester - I

**CHI-130:** Molecular Symmetry & Chemistry of p-block elements (4 credits)

### **SECTION-I:** Molecular Symmetry and its Applications

(2 Credits, 24 L, 6 T)

- (a) **Definitions and Theorems of Group Theory:** Defining properties of a group, group multiplication table, some examples of group, subgroups, classes
- **(b) Molecular Symmetry and Symmetry Groups:** Symmetry elements and operations, Symmetry planes and reflections, the inversion centre, proper axes and proper rotations, improper axes and improper rotation, products of symmetry operations, equivalent symmetry elements and equivalent atoms, general relations symmetry elements and symmetry operations, symmetry elements and optical isomerism, symmetry point groups, classes of symmetry operations, classification of molecular point groups.
- (c) Representations of Groups: Matrix representation and matrix notation for geometric transformation, The Great Orthogonality Theorem and its consequence, character tables (No mathematical part)
- (d) Group theory and quantum mechanics: Wave function as basis for irreducible representations
- (e) Symmetry Adapted Linear Combinations: Projection operators and their use of construct SALC (Construction of SALC for sigma bonding for molecules belonging point groups:  $D_{2h}$ ,  $D_{3h}$   $D_{4h}$ ,  $C_{4v}$ , Td, Oh, normalization of SALC.
- **(f) Molecular Orbital Theory:** Transformation properties of atomic orbital, MO's for Sigma bonding ABn molecules, tetrahedral AB<sub>4</sub> and Oh AB<sub>6</sub> cases.

#### **References:**

1) Chemical Applications of Group Theory, 3<sup>rd</sup> Ed<sup>n</sup>., Author - F. A. Cotton (Wiley, New York)

- 2) Symmetry and spectroscopy of molecules, 2<sup>nd</sup> Ed. 2009; K. Veera Reddy, (New Age International Publication)
- 3) Group Theory and its Chemical Applications, P.K. Bhattarchrya

#### **Section-II: Chemistry of Main group elements**

(2 Credits, 24 L, 6 T)

- 1. Hydrogen and its compounds: Hydrides: Classification, electron deficient, electron precise and electron rich hydrides. PH<sub>3</sub>, SbH<sub>3</sub>, AsH<sub>3</sub>, Selenides, Tellurides (2 L)
- 2. Alkali and alkaline earth metals: Solutions in non-aqueous Media, Application of crown ethers in extraction of alkali and alkaline earth metals (2 L)
- 3. Organometallic Compounds of Li, Mg, Be,: Classification, Synthesis, Properties, Uses and Structure (3 L)
- Boron Group: Boron Hydrides, preparation, structure and Bonding with reference to LUMO, HOMO, interconversion of lower and higher boranes, Metalloboranes, Carboranes, Reactions of Organoboranes
   (4 L)
- 5. Carbon Group: Allotropes of Carbon, C<sub>60</sub> and compounds (fullerenes), Intercalation compounds of Graphite, Carbon nanotubes, synthesis, properties, structure-single walled, multi walled, applications (2 L)
- 6. Organometallic compounds of Si, Sn, Pb, Ga, As, Sb, Bi. Structures, synthesis, (3 L) Reactions
- 7. Nitrogen Group: Nitrogen activation, Boron nitride, Oxidation states of nitrogen and their interconversion, PN and SN Compounds, NOx and their redox chemistry (3 L)
- Oxygen Group: Metal Selenides and Tellurides, oxyacids, and oxoanions of sulphur & nitrogen. Ring, Cage and Cluster compounds of p-block elements. Silicates, including
   Zeolites
- 9. Halogen Group: Interhalogens, pseudo-halogen, Synthesis, Properties and Applications,Structure, Oxyacids and Oxoanions of Halogens, Bonding (2 L)

#### References:

- 1) Inorganic Chemistry : Shriver & Atkins (4<sup>th</sup> edition 2003, Oxford)
- 2) Concise Inorganic Chemistry, J. D. Lee, Fourth Edn.(Chapman and Hall)

- 3) Inorganic chemistry: principle of structures and reactivity, Huheey, Keiter, Keiter, Medhi, Pearson Education, 4<sup>th</sup> Edn. (2007).
- 4) Inorganic Chemistry: Catherine Housecroft
- 5) Inorganic Chemistry: Messler & Tarr, Pearson Publishers 3rd Edition
- 6) Organometallic Chemistry-A Unified Approach: R. C. Mehrotra & A. Singh

## **Organic Chemistry**

### Semester - I

### CHO-150: Basic organic chemistry

(4 Credits)

Section-I

(2 credits, 24 L, 6 T)

#### 1. Structure and reactivity:

(10 L)

- a) Chemical bonding and basis of reactivity- Chemical bond, delocalization, conjugation, resonance, hyperconjugation, tautomerism, inductive effects.
- b) Acidity and basicity: various structural effects, hard and soft acid and base concept.
- c) Aromaticity: Benzenoid and non-benzenoid compounds, Huckels rule, antiaromaticity, Application to carbocyclic and heterocyclic systems, annulenes, azulenes, current concepts of aromaticity.
- d) Structure and stability of reactive intermediates, carbenes, nitrenes, carbocations, carbanions and free radicals.

### 2. Stereochemistry: (14 L)

- a) Sterochemical principles, enantiomeric relationship, distereomeric relationship, R and S, E and Z nomenclature in C, N, S, P containing compounds, Prochiral relationship, stereospecific and stereoselective reactions, optical activity in biphenyls, spiranes, allenes.
- b) Conformational analysis of cyclic and acyclic compounds.

#### **Section-II**

#### 1. Organic reactions:

(2 credits, 24 L, 6 T)

#### a) Substitution reaction:

(10 L)

Aliphatic nucleophilic substitution- $S_N1$ ,  $S_N2$  mechanism, NGP by pi and sigma bonds, classical and non-classical carbocations, phenonium ions, norbornyl system, carbocation rearrangement in NGP, SNi mechanism, nucleophilic substitution in allylic,trigonal and vinylic carbon.

Effect of structure, nucleophile, leaving group and solvent on rate of  $S_N1$  and  $S_N2$  reactions, ambident nucleophile and regioselectivity.

#### b) Aromatic Electrophilic substitution

(4 L)

Arenium ion mechanism, orientation and reactivity, energy profile diagram, ortho, para, ipso attack, orientation in other ring systems, six and five membered heterocycles with one hetero atom.

Important reactions like Friedel crafts alkylation and acylation, Nitration, halogenation, formylation, chloromethylation, sulphonation, diazonium coupling.

#### **Aromatic nucleophilic substitution**

(2 L)

 $S_NAr$ ,  $S_N1$ , Benzyne and  $S_NR1$  reactions, reactivity: effect of substrate structure, leaving group and attacking nucleophile.

#### c) Addition reactions

(4 L)

Addition to C-C multiple bonds - mechanism and stereochemical aspects of addition reaction involving electrophile, nucleophile and free radicals, Regio and chemo selectivity, orientation and reactivity, conjugate addition.

#### d) Elimination reactions

(4 L)

E1, E2, E1cb mechanisms, orientation and stereochemistry in elimination reaction, reactivity effect of structure, attacking and leaving group, competition between elimination and substitution, syn eliminations.

#### **References:**

- 1. Organic Chemistry-by J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford)
- 2. Advanced Organic Chemistry –by J. March 6<sup>th</sup> Edition
- 3. Advanced Organic Chemistry (part A) -by A. Carey and R.J. Sundberg
- 4. Stereochemistry of carbon compound-by E.L. Eliel
- 5. Stereochemistry of organic compound-by Nasipuri
- 6. Guide book to Reaction Mechanism –Peter Sykes

## **General Chemistry**

#### Semester – I

## CHA-190: Safety in Chemical Laboratory and Good Laboratory Practices (4 Credits, 48 L, 12 T)

#### Section-I

# 1. History and importance of safety and health in Laboratory Importance of Safety and security, responsibility and accounting for safety, types of hazards and risk in chemical laboratory, Moral legal and financial reasons, Introduction

to different types of Hazards

Ref. 1 Page 1-11

#### 2. Establishing Effective chemical safety and security management

2L

Introduction, responsibility of laboratory safety and security, ten step to creating an effective laboratory chemical safety and security management safety Ref.1 Page 15-19

#### 3. Personnel protective and other safety equipments

3L

Personnel clothing, foot protection, eye and face protection, safety shield, fire safety equipments, heat and smoke detector, respirators, safety showers, eye wash unit Ref. 1 Page 215-220

#### 4. Assessing routes of exposer for toxic chemicals

4L

Inhalation, contact with skin and eye, ingestion, assessing risk with acute toxicology, specific chemical hazard, First aid for contact of different chemicals on skin, eyes, and inhalation ingestion.

Ref. 1 Page 201-210.

#### 5. Assessing hazards and risk in the laboratory

**7**L

Introduction, consulting source of information, evaluating the toxic risk of laboratory chemicals, assessing flammable, reactive and explosive hazards, Assessing physical hazards, assessing bio hazards

Ref. 1 Page 73-90

#### 6. Managing Chemicals

4L

Introduction, green chemistry for every laboratory, purchasing chemicals, inventory and tracking of chemicals, storage of chemicals, transfer, transport, shipment of chemicals. Ref. 1 Page 92-104

#### **Section-II**

#### 7. Working with Chemicals

**8T** 

Introduction, careful planning, general procedure for working with hazardous chemicals, working with substance of high toxicity, working with bio hazards material, working with flammable chemicals, working with highly reactive or explosive chemicals Ref. 1 Page 107-125

#### 8. Working with laboratory equipments

3L

Introduction, working with electrically powered equipment, working with compressed gases, working with high and low pressure and temperatures.

Ref. 1 Page 137-143

#### 9. Managing chemical waste

5L

Introduction, identifying waste and its hazards, collecting and storing waste, treatment and hazard reduction, disposal options Ref. 1 Page 152-161.

#### 10. Introduction to Good Laboratory Practices and its applications

4L

General introduction, Drug development process and non-regulated vs. regulated area, GMP, Introduction to GLP and its applications, GLP Training, introduction, Fundamental points of GLP

Ref. 2 Page 9-18

#### 11. Rules for conduct of studies

4L

General aspects, Study plan of protocol, Content of the protocol, Identification, Approval of protocol, protocol amendment, Standard operating procedures, SOP system overview Ref. 2 Page 27-36

Ref. 1 Chemical Laboratory Safety and Security, A Guide Prudent Chemical Management Edited by Lisa Moran and Tina Masciangioli Available Online www.nap.edu (Free)

Ref. 2 Hand Book, Good Laboratory Practice (GLP) Available Online (Free)

## **Physical Chemistry**

#### Semester – II

#### **CHP-210: Fundamentals of Physical Chemistry-II**

(4 Credits)

#### **SECTION-I**

(2 Credits, 24 L, 6 T)

#### **Molecular Spectroscopy**

- 1) Recapitulation:-Width and intensity of spectral transitions, Fourier transform, microwave spectroscopy, rotation spectra of di and ply atomic molecules, Stark effect (04 L)
- 2) Infra red spectroscopy: Harmonic and an harmonic oscillator, vibrational spectra of di and poly- atomic molecules, coarse and fine structure, Nuclear spin effect, application, (05 L)
- Raman Spectroscopy: Introduction, Rotational Raman- spectra, Vibrational Raman , Spectra, polarization of light and Raman effect, structure elucidation from combined Raman and IR spectroscopy, applications in structure elucidation. (05 L)
- 4) Electronic spectroscopy of molecules: Born Oppenheimer approximation, electronic spectra of diatomic molecules, vibration, al coarse structure, rotational fine structure dissociation energy and dissociation products, electronic structure of diatomic molecules, molecular photoelectron spectroscopy, and application. (06 L)
- 5) ESR and Mossbauer spectroscopy applications. (02 L)
- 6) Principles of NMR Chemical applications of PMR in structure elucidation. (02 L)

#### Reference:

Fundamentals of molecular spectroscopy: C.N. Banewell and E.Mc. Cash (Fourth edition).

#### **SECTION-II**

(2 Credits, 24 L, 6 T)

#### **Nuclear and Radiation Chemistry**

Radio Chemistry: recapitulation – type of radioactive decay, Decay Kinetics, Detection
 & measurement of radiation (G.M. & Scintillation counter)

- 2) Elements of radiation chemistry Radiation chemistry, interaction of radiation with miller, passage of nucleolus through matter, interaction of radiation with matter, Units. for measuring radiation absorption, Radiation dosimetry, Radiolysis of water, free radiation in water Radiolysis, Radiolysis of some aqueous solution. (06 L)
- 3) Nuclear Reactor: The fission energy, The Natural uranium reactor, the four factor formula- The reproduction factor K, the classification of reactor. Reactor power, Critical size of thermal reactor, excess reactivity & control, the Breeder reactor, The Indians nuclear energy programme, Reprocessing of spent fuel, Recovery of Uranium & Plutonium, Nuclear waste management, Natural nuclear reactor. (06 L)
- 4) Isotopes for nuclear reactors. Isotope separation, separation of selected isotopes, Plutonium. (03 L)
- 5) Applications of radioactivity: Typical reaction involved in preparation of radio isotopes: <sup>3</sup>H, <sup>14</sup> C, <sup>22</sup>Na <sup>32</sup>P <sup>35</sup>S, and I <sup>127</sup> General principles of using radioisotopes. Physical constants Diffusion coefficients, surface area, solubility. Analytical applications-neutron activation analysis, dilution analysis, radiometric titration. Industrial applications radiation guaging, friction and wear out, gamma radiography. (06 L)

#### Reference Books

- 1. Elements of Nuclear chemistry H.J. Arnikar, fourth edition wiley Estern Ltd.
- 2. Source book of atomic energy S. Glasstanc, D. Van Norton Company
- 3. Chemical applications of radioisotopes H.J. M. Brown Buffer & Jammer Ltd.

## **Inorganic Chemistry**

#### Semester – II

### CHI-230: Coordination and Bioinorganic Chemistry (4 Credits)

**SECTION-I:** Coordination Chemistry (2 Credits, 24 lectures, 6 T)

- 1. Concept & Scope of Ligand Fields, Free ion Configuration, Terms and States, Energy levels of transition metal ions, free ion terms, term wave functions, spin-orbits coupling. (4 L)
- Ligand Field Theory of Coordination Complexes (7 L)
   Effect of ligand field on energy levels of transition metal ions, weak cubic ligand field effect on Russell- Saunders terms, strong field effect, correlation diagrams, Tanabe- Sugano Diagrams, Spin-Pairing energies.
- 3. Electronic spectra of Transition Metal Complexes (7 L) Introduction, Band intensities, band energies, band width & shapes, spectra of 1<sup>st</sup>, 2<sup>nd</sup> & 3rd row ions and rare earth ion complexes, spectrochemical & nephlauxetic series, charge transfer & luminescence, spectra, calculations of Dq, B, β parameters.
- 4. Magnetic Properties of Coordination Complexes (6 L)
  Origin magnetism, types of magnetism, Curie law, Curie-Weiss Law, Magnetic properties of complexes-paramagnetism 1st & 2nd Ordered Zeeman effect, quenching of orbital angular momentum by Ligand fields, Magnetic properties of A, E & T ground terms in complexes, spin free spin paired equilibria.

#### **References:**

- 1. Ligand field theory & its applications: B.N. Figgis & M.A. Hitachman (2000) Wiely VCH Publ.
- 2. Symmetry and spectroscopy of molecules, Second Ed<sup>n</sup>, by K. Veera Reddy, New Age International Publication, 2009.
- 3. Elements of magnetochemistry, R. L. Datta and Syamal, Second Ed<sup>n</sup>, Afiliated East West Press Pvt. Ltd. 2007.

#### **Section-II: Bioinorganic Chemistry**

(2 Credits, 24 Lectures, 6 T)

1. Overviews of Bioniorganic Chemistry

(1 L)

- Principles of Coordination Chemistry related to Bioinorganic Research and Protein,
   Nucleic acids and other metal binding biomolecules.
- 3. Biochemistry of Na, K and Ca w.r.t. Na/K pumps, Calmodulin and blood coagulation.

(8 L)

- 4. Biochemistry of following elements:
  - (a) Iron: Ferritin, Transferrin, Fe-S clusters, Porphyrin based systems

(6 L) (2 L)

(b) Manganese: Photosynthesis

## Reference Books:

- 1. Principle of Bioinorganic Chemistry: S.J. Lippard and J,M. Berg
- 2. Bioinorganic Chemistry: Inroganic Elements in Chemistry of Life: W.Kaim and B. Schwederski
- 3. Bioinorganic Chemistry: Bertini, Gray, Lippard and Valentine
- 4. Bioinorganic Chemistry: R.J.P. Willams
- 5. Bioinorganic Chemistry: Robert Hay
- 6. Bioinorganic Chemistry: M.N. Hughes

## **Organic Chemistry**

## Semester – II

СНО	CHO-250: Synthetic organic chemistry and spectroscopy (4 Credits					
SE	CTION – I: Synthetic Organic Chemistry	(2 Credits, 24 L, 6 T)				
1.	Oxidation reactions:					
	CrO <sub>3</sub> , PDC, PCC, KMnO <sub>4</sub> , MnO <sub>2</sub> , Swern, SeO <sub>2</sub> , Pb(OAc) <sub>4</sub> , Pd-C	, OsO <sub>4</sub> , m-CPBA, O <sub>3</sub> ,				
	NaIO <sub>4</sub> , HIO <sub>4</sub>					
2.	Reduction reactions:	(4 L)				
	Boranes and hydroboration reactions,					
	MPV reduction and reduction with $H_2/Pd-C$ , Willkinsons catalyst,	DIBAL and Wolff				
	Kishner reduction.					
3.	Rearrangements:	(6 L)				
	Beckmann, Hofmann,, Curtius, Smith, Wolff, Lossen, Bayer-villig	ger,				
	Sommelet, Favorskii, Pinacol-pinacolone, Benzil-benzilic acid, Fri	ies.				
4.	Ylides:	(4 L)				
	Phosphorus, Nitrogen and Sulphur ylides					
5.	Addition to carbonyl group:	(4 L)				
	Grignard, organo zinc, organo copper, organo lithium, reagents to	carbonyl and				
	unsaturated carbonyl compounds.					
	SECTION-II: Spectroscopy (2 Cre	edits 24 Lectures, 6T)				
	a) UV: Factors affecting UV absorption and interpretation of UV s	spectra (2 L)				
	b) IR: Basic ideas about IR frequencies, interpretation of IR spectr	a (4 L)				
	c) PMR: Fundamentals of PMR, factors affecting chemical shift, in	tegration				
	coupling (1 <sup>st</sup> order analysis)	(8 L)				
	d) Introduction to CMR and mass spectrometry	(4 L)				
	e) Problems on UV, IR and PMR	(6 L)				

#### **References:**

- 1. Organic Chemistry J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford)
- 2. Modern Synthetic reactions- H.O. House
- 3. Organic Synthesis M.B. Smith
- 4. Advanced Organic Chemistry (part A & B)- A. Carey and R.J. Sundberg
- 5. Stereochemistry conformations and mechanism by P.S. Kalsi
- 6. Organic chemistry –by Cram, Hammond, Pine and Handrickson
- 7. Introduction to spectroscopy D.l. Pavia, G.M. Lampman, G.S. Kriz, 3<sup>rd</sup> Edition
- 8. Spectroscopic methods in organic melecules D.H. William & I Flemming Mc Graw Hill
- 9. Mechanism and Structure in Organic Chemistry E.S. Gould

## **General Chemistry**

#### Semester - II

#### CHA-290: General Chemistry – II

(Any two parts except B)

(4 Credits)

PART-A: Modern Separation Methods and Hyphenated Techniques (2 Credits, 24 L, 6 T)

#### 1. Mass Spectrometry

(8 L)

Principle, Instrumentation, Ionization methods- Electron bombardment ionization, Arc and spark ionization, Photo-ionization, Thermal ionization, Chemical ionization, Mass analyzers-Magnetic, Double focusing, Time of flight, Quadrupolar, Ion cyclotron resonance analyzer, Correlation of mass spectra with molecular structure and molecular weight, Isotopic Abundances, Fragmentation patterns, Quantitative analysis, Applications and Problems. Fourier transform mass spectrometry, Tandem mass spectrometry, inductively coupled Plasma-mass spectrometry,

#### Ref. 1, Pages 647-696; Ref. 2, Pages 465-506

#### 2. Gas Chromatography

(8 L)

Theory and Instrumentation of GC, Sample injection- Split and splitless injection, Column types, Solid/Liquid Stationary phases, Column switching techniques, Basic and specialized detectors, elemental detection, chiral separations, , Gas chromatographs and chemical analysis, Interfacing of gas chromatography with mass spectrometry, Applications of GLC, Use of GC-MS, High Speed gas chromatography, Gas-solid chromatography and problems,

#### Ref. 2, Pages 540-569; Ref. 3, Pages 125-143; Ref. 4, Pages 947-970.

#### 3. High Performance Liquid Chromatography (HPLC)

(8 L)

Theory and instrumentation of HPLC, Optimization of column performance, Gradient elution and related procedures, Derivatization, Mobile phase delivery system, sample injection, separation column, detectors, Interfacing HPLC with mass spectrometry, Structure types of

column packing, adsorption chromatography, Bonded phase chromatography, reverse phase chromatography, ion-pair chromatography, ion exchange chromatography, size exclusion chromatography, GC-MS and LC-MS, Applications and Problems.

#### Ref. 2: Pages 580-650, Ref. 4: Pages 974-992.

#### **References:**

- 1. Introduction to Instrumental Analysis, R. D. Braun, Mc Graw-Hill. Inc. 1987.
- 2. Instrumental Methods of Chemical analysis, H. H. Willard, L. L. Merritt Jr., J. A. Dean & F. A. Settle Jr., 6th Edition, Wadsworth Publishing Company, USA,1986
- 3. Handbook of Instrumental Techniques for Analytical Chemistry, F. A. Settle editor, Prentice Hall Inc. A Simon and Schuster Company, New Jersey, 1997.
- 4. Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, 7th Edition, Thomson Asia Pte. Ltd, Singapore, 2004

## PART-B: (Compulsory for Drug Chemistry Students and Students from other disciplines also can opt for it)

#### **Basic Biochemistry**

(4 Credits, 48 L, 12 T)

- 1. Introduction to Biochemistry: Scope of the subject in pharmaceutical sciences, Biochemical reactions, Highlights of prokaryotic and Eukaryotic cell metabolism.
- 2. Biochemical Morphology: Prokaryotes and Eukaryotes, Cell structure, sub-cellular components: Nucleus, plasma membranes, endoplasmic reticulum, Lysosome, Peroxisomes, Golgi apparatus, and Mitochondria.
- 3. Biomembrane: Structure, functions and composition, Model proposed, Function and properties of membrane, Transport hypothesis, Active and passive facilitated transport, Na+, K+, H+, pumps, glucose transport, Excitable membrane, drug transport.

#### 4. Biomolecules:

Proteins: Introduction, functional, classification of amino acids, classification, physicochemical properties, Optical activity, Reaction with ninhydrin, Formaldehyde, Aminoacids, Essential and non essential amino acids, efficacy, structure, peptide bond, end group analysis, Helix, B-sheet structure, tertiary, quaternary structure, globular protein, fibrous protein, amino acid therapy, Protein engineering

Carbohydrates: complex carbohydrate, structure of Chitin, Starch, Glycogen + Metabolism

Lipids: definition, classification, functions, types of fatty acids, and its biological role and metabolism.

5. Enzymes: Introduction, classification according to the reaction catalysis and source) structure of enzyme, co factures, active sites, Binding sites, Km, Vmax, Enzyme kinetics, Double reciprocal plot, effect of substrate, pH ionic strength, Concentration, Temperature on the rate of enzyme reactions, Enzyme inhibition(competitive, uncompetitive, non competitive and irreversible), Enzyme biotechnology. Manufacturing of medicinal compounds by enzymatic reactions, Penicillin acylase for the production 6-APA, Therapeutical uses of enzymes.

#### **References:**

- 1. Principals of biochemistry, Albert Lehninger (CBS Publisher and Distributers Pvt. Delhi.
- 2. Biochemistry Lubert Stryer, W. H. (Freeman and company New York)
- 3. Harper's Biochemistry by R.K. Murray, D. I. Granner, P. A. Mayes, (Prentice Hall International Inc.)
- 4. Practical Clinical Biochemistry, Harold Varley, (CBS Publisher and Distributers Pvt. Delhi.
- 5. Molecular Biology, J.D. Watson (The Benjamin/ Cumming Company, Inc.)

#### **PART- C: Concept of Analytical Chemistry**

(2 Credits, 24 L, 6 T)

#### 1. Data Handing and Spreadsheets in Analytical Chemistry

(6 L)

Accuracy and Precision, classification of errors, Significant figures, rounding off, ways of expressing accuracy, Mean Deviation, Average Deviation, RMD, Standard Deviation Propagation of errors, Confidence limits, Tests of Significance, Rejection of results and Problems.

#### Ref. 2: Pages 65-99.

#### 2. Sampling, Standardization and Calibration

(8 L)

Analytical Samples and Methods of Sampling, Sample Handling, Gross sample, Preparation of Laboratory samples, Automated Sample Handling, Comparisons with standard and Numerical Problems.

#### Ref. 1: Pages 175-200.

#### 3. Introduction to analytical separations

(8 L)

Separation by precipitation, separation of species by distillation, separation by extraction, separation by ion exchange chromatography and problems.

#### Ref. 1: Pages 906-946

#### References:

- 1. Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, 5th Edition, Thomson Asia Pte. Ltd, Singapore, 2004.
- 2. Analytical Chemistry, G.D. Christian, 6 th Edition.

#### **PART- D: Industrial Methods of Analysis**

(2 Credits, 24 L, 6 T)

#### 1. Chemometrics: (10 L)

Concentration of solution based on volume and mass unit, calculations of ppm, ppb and dilution of the solutions, Concept of mmole, Stoichiometry of chemical reactions, Concept of gmole, Limiting reactants, theoretical and practical yield, solubility and solubility equilibria. Concept of formation constant, Stability and instability constants, stepwise formation constants and Numerical problems.

#### 2. Quality in Analytical Chemistry

(6 L)

Quality systems in chemical laboratories, cost and benefits of quality system, types of quality standards for laboratories, total quality management, quality audits, and qualities reviews, responsibility of laboratory staff for quality and problems.

#### 3. Process Instruments and Automated Analysis

(8 L)

Introduction, industrial process analyzer, methods based on bulk properties, continuous online process control, automatic chemical analyzers, automatic elemental analyzers, Numerical problems.

#### Ref 3: Pages: 786-828.

#### **References:**

- 1. Vogel's Text book of Quantitative Analysis.
- 2. Analytical Chemistry, G.D. Christian, 6 th Edition.
- 3. Instrumental Methods of Chemical analysis, H. H. Willard, L. L. Merritt Jr., J. A. Dean & F. A. Settle Jr., 6th Edition, Wadsworth Publishing Company, USA,1986

## PART- E: Organometallic and Inorganic Reaction Mechanism (2 Credits, 24 L, 6 T) (Recommended for M. Sc. other than Inorganic specialization)

#### 1) Organometallic Chemistry

(8 L)

Organic ligands and nomenclature, 18 electron rule: counting electrons, ligands having extended pi system, bonding between Metal Atoms and organic pi systems: linear pi system, cyclic pi system, spectral analysis and characterization of organometallic complexes: IR and NMR, examples.

#### 2) Organometallic Reactions and Catalysis

(8 L)

(8L)

Reactions involving gain and loss of ligands: ligand dissociation and substitution, oxidative addition, reductive elimination, nucleophelic displacement, **r**eactions involving modification of ligands: insertion, carbonyl insertion, 1-2 insertion, hydride elimination, abstraction, organometallic catalysis: Hydroformylation, Monsanto acetic acid process, Wacker Process, Hydrognation by Willkinsons catalyst, Olefin metathesis, heterogeneous catalysis: Ziegler Natta Polymerization, Water gas reduction.

#### 3) Coordination Compounds: Reactions and Mechanism

History and principles, Substitution reactions: Inert and labile complexes, mechanism of substitution, Kinetics Consequences of reaction pathway: dissociation, interchange, association, Experimental evidences in Octahedral Substitution: dissociation, linear free energy relationship, associative mechanism, the conjugate base mechanism, the kinetic chelate effect, Stereochemistry of reactions: substitution in trans complexes, substitution in cis complexes, isomerisation of chelate rings, substitution reactions in Sq. Pl. Complexes.

#### Reference Book:

Inorganic Chemistry: Gary Miessler and Donald A. Tarr, Third Ed., Pearson (Chapter-12, 13 and 14 pages: 422 to 561)

#### **Part F: Mathematics for Chemists**

(2 Credit; 24 L, 6 T)

#### (Recommended for M. Sc. other than Physical Chemistry specialization)

- Functions: Differential and integral calculus, limits, derivatives, physical significance, basic
  rules of differentiation, maxima and minima, application is chemistry, exact and inexact
  differentiation, Taylor & McLaurin Theorem, curve sketching, partial differentiation, rules of
  integration, separation of variable, substitution, partial function method to solve to indefinite
  integrals in chemistry. (14 L)
- Differential Equations: Separation of variables, homogeneous, exact, linear equations of second order, series solution method.
- Vectors Matrices, and Determinants: (4 L)
   Vectors, dot, Corss and triple products, introduction to matrix algebra, addition and multiplication of matrices, inverse, adjoins and transport of matrices, unit and diagonal matrices.

#### References:

- 1) Chemical Maths Book, E. Steiner, Oxford University Press (1996).
- 2) Mats For Chemists Vol 1 and 2, Martin MCR Cockett and G. Doggett, Cambridge (2003).
- 3) Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill (1972)

## Part G: Pericyclic reactions, Photochemistry and Free radicals (2 Credit; 24 L, 6 T) (Recommended for M. Sc. other than Organic Chemistry specialization)

#### 1. Pericyclic reactions (10 L)

Electrocyclisation, cycloaddition, sigmatropic and Alder-ene reactions. Analysis of pericyclic reactions by construction of correlation diagrams and by FMO approach.

#### 2. Free radicals (6 L)

Generation, stability and general reactions like displacement, addition and rearrangements.

3. Photochemistry (8 L)

Basic concepts in Photochemistry, Jablonski diagram, quenching, triplet excitation, photosensitization, quantum yield, photochemistry of carbonyl compounds (photoreduction, photoenolization, Norrish type I and II) and benzene derivatives.

#### **References:**

- 1. Conversation of orbital symmetry Woodward and Hoffmann
- 2. Organic Chemistry Morrison and Boyd
- 3. Organic Chemistry Warren, Clayden, Greeves and Wothers
- 4. Advanced Organic Chemistry Carey, Sandburg Vol. A.
- 5. Organic reactions and Orbital Symmetry T. L. Gilchrist and R. C. Storr
- 6. Excited states in Organic Chemistry J. D. Coyle and J. A. Barltrop
- 7. Orbital Symmetry A problem solving approach. R. F. Lehr and A. P. Marchand
- 8. Principles of Organic Synthesis Norman, Coxon

## M.Sc.-I: Practical

## **CHP-107: Physical Chemistry Practicals**

(6 Credits)

#### A) Conductometry: (Any four)

- 1. Study the Hydrolysis of NH<sub>4</sub>Cl or CH<sub>3</sub>COONa or aniline hydrochloride.
- 2. Determination of equivalent conductance at infinite dilution and dissociation constant of acetic acid.
- 3. Study the second order velocity constant of the hydrolysis of ethyl acetate by sodium hydroxide.
- 4. Determination of G, H, and S of silver benzoate by conductometry.
- 5. Determination of critical micellar concentration (CMC) and G of micellization of sodium dodecyl sulphate (SDS).
- 6. Determination of concentrations of strong acid and weak acid present in the mixture by titration with strong base.

#### **B) Potentiomerty: (Any four)**

- 1. Determination of stability Constant of a complex ion.
- 2. Determination of Solubility and solubility product of a sparingly soluble salt.
- 3. Estimation of amount of halides present in the mixture.
- 4. Determination of concentrations of strong acid and weak acid present in the mixture by titrating with strong base.
- 5. Determination of concentrations of reductant or oxidant by redox titration.

#### C) pH metry: (Any two)

- 1. Determination of the acid and base dissociation constant of an amino acid and hence the isoelectric point of the acid.
- 2. Determination of dissociation constants of tribasic acid (phosphoric acid)
- 3. Determination of Hammett constant of o-, m-, p- amino/nitro benzoic acid.

#### D) Polarography:

1. Determination of half wave potential ( $E_{1/2}$ ) and unknown concentration of an ion. 2. Amperometric titration of Pb(NO<sub>3</sub>)<sub>2</sub> with K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>.

#### E) Colorimetry/Spectrophotometry: (Any two)

1. Simultaneous determination of cations from the mixture.

- 2. Determination of amount of copper by photometric titration with EDTA.
- 3. Study the kinetics of iodination of acetone spectrophtometrically.

#### F) Radioactivity: (Any two)

- 1. Estimation of Manganese in tea leaves by Neutron Activation Analysis.
- 2. Determination of half-life of a radioactive nuclide and counting errors.
- 3. Determination of  $E_{max}$  of  $\beta$  radiation and absorption coefficients in Al.

#### **G)** Chemical Kinetics: (Any three)

- 1. Study of Kinetic decomposition of diacetone alcohol by dilatometry.
- 2. Determination of individual orders of iodide and persulphate ions and overall order of oxidation reaction of iodide ion by persulphate ion.
- 3. Investigation of influence of ionic strength on rate constant (Brönsted primary salt effect).
- 4. Determination of temperature coefficient and energy of activation of acid catalyzed ester hydrolysis reaction.

#### H) Non-Instrumental: (Any five)

- 1) Determination of surface excess of amyl alcohol or TX-100 surfactant by Capillary rise method.
- 2) Statistical treatment of experimental data.
- 3) Determination of molecular weight by steam distillation.
- 4) Determination of glycerol radius by viscosity.
- 5) Determination of partial Molar Volume (Polynometry) and the densities of a series of solutions and to calculate the molar volumes of the components.
- 6) Analysis of crystal structure from single crystal X-ray pattern.

#### **References:**

- 1. Practical physical chemistry, A. Findlay, T.A. Kitchner (Longmans, Green and Co.)
- 2. Experiments in Physical Chemistry, J.M. Wilson, K.J. Newcombe, A.r. Denko. R.M.W. Richett (Pergamon Press)
- 3. Senior Practical Physical Chemistry, B.D. Khosla and V.S. Garg (R. Chand and Co., Delhi.).
- 4. Experimental Physical Chemistry by D. P. Shoemaker, Mc. Growhill, 7<sup>th</sup> Edition, 2003.
- 5. Physical chemistry by Wien (2001)
- 6. Practical physical chemistry, B. Vishwanathan and P.S. Raghavan, 2<sup>nd</sup> edition, (2012)

7. Experimental Ph	iysical c	chemistry,	V.D.	Athawale,	Parul Mathur,	New	age	International
publishers.								

## **CHI-107: Inorganic Chemistry Practical**

(6 Credits)

#### Part-I: Ore analysis (Any Two) (Ref. -1)

a. Analysis of Pyrolusite ore.

Determination of (i) Silica and (ii) Manganese

b. Analysis of Chalcopyrite ore.

Determination of (i) Copper and (ii) Iron

c. Analysis of hematite ore.

Determination of (i) Silica and (ii) Iron

#### Part-II: Alloy Analysis (Any Two) (Ref. -1)

- a. Determination of tin and lead from solder.
- b. Determination of iron and chromium from mild steel.
- c. Determination of copper and nickel from cupronickel.

#### **Part-III: Inorganic Synthesis and Purity (Any five)**

(Ref. - 2)

#### Part A: Five preparations

#### Part B; Purity determination of above preparations

- a. Mn(acac)<sub>3</sub>
- b. Chloro penta-ammine cobalt (III) chloride
- c. Nitro penta-amminecobalt (III) chloride
- d. Nitrito penta-amine cobalt (III) Chloride.
- e. Potassium tri-oxalato aluminate
- f. Tris(ethylene di ammine) Ni(II) thiosulphate.
- d. Bis[TrisCu(I)thiourea]

[Part A and B shold be treated as separate experiments]

#### **Part-IV: Ion – exchange chromatography** (Any one experiment)

(Ref. -1 and 3)

- a) Separation of mixture of Zn(II) and Cd(II) using Amberlite IRA 400 anion exchanger and quantitative estimation of separated ions Zn(II) and Cd(II)
- b) Separation of mixture of Zn(II) and Mg(II) using Amberlite IRA 400 anion exchanger and quantitative estimation of separated ions Zn(II) and Mg(II)

#### **Part-V: Spectrophotometry** (any two experiments)

- a. Estimation of phosphate from waste water by calibration curve method4)
- b. Determination of equilibrium constant of M-L systems Fe (III) Salicylic acid or Fe(III)–Sulphosalicylic acid or Fe(III)– $\beta$ –resorcilic acid by Job's continuous variation

method. (Ref.-3)

c. Determination of iron by solvent extraction techniques in a mixture of Fe(III) +AL(III) or Fe(III) + Ni(III) using 8-hydroxyquinoline reagent.
 (Ref. -1)

or

c) Determination of Cu(II) by solvent extraction as Dithiocarbamate/8-Hydroxyquinoline complex (Ref-1,3)

#### Part-VI: Inorganic characterization techniques (any one of the following)

- a. Solution state preparation of [Ni(en)<sub>3</sub>]S<sub>2</sub>O<sub>3</sub>, [Ni(H<sub>2</sub>O)<sub>6</sub>]Cl<sub>2</sub>, [Ni(NH<sub>3</sub>)<sub>6</sub>]Cl<sub>2</sub>. Record absorption spectra in solution of all three complexes and analyse it. Arrange three ligands according to their increasing strength depending on your observations. (Ref. -5)
- b. Determination of magnetic susptibility ( $\chi_g$  and  $\chi_m$ ) of mercury tetracyanato cobalt or Fe(acac)<sub>3</sub> or Ferrous ammonium sulfate by Faraday or Gouy method.

(R ef. -3)

#### Part-VII: Synthesis of Nanomaterials (any one of the following)

a) Synthesis of nano size ZnO, its characterization by UV-Visible spectroscopy and removal

of dye by ZnO-photocatalysis
(
Ref-2)

b) Synthesis of nano size  $\alpha\text{-Fe}_2\text{O}_3$  and study of adsorption of phosphate on it

4 TITT C 1 4 4 4 6 11 1 1 1

**Part-VIII: Conductometry** (any one of the following).

**Ref-2**)

- a) Verification of Debye Huckle theory of ionic conductance for strong electrolytes KCl,BaCl<sub>2</sub> K<sub>2</sub>SO<sub>4</sub>, K<sub>3</sub>[Fe(CN)<sub>6</sub>] (Ref. -3)
- b) Structural determination of metal complexes by conductometric measurement. (Ref-3)
- c) To study complex formation between Fe(III) with sulfosalicylic acid by conductometry (Ref-3).

#### **Part-IX:** (any one of the following)

- a) Synthesis and photochemistry of  $K_3[Fe(C_2O_4)_3]$  3H<sub>2</sub>O. (**Ref-4**)
- b) Kinetics of substitution reaction of [Fe(Phen)<sub>3</sub>]<sup>2+</sup> (**Ref-3**)

#### Part-X: Table work

a) Data analysis, error analysis, least squares method.

(Ref-3)

#### **Reference Books:**

- 1) Text book of Quantitative Analysis, A.I. Vogel 4<sup>th</sup> Edn. (1992).
- 2) Experimental Inorganic Chemistry, Mounir A. Malati, Horwood Series in Chemical Science (Horwood publishing, Chichester) 1999.
- 3) Experiments in Chemistry, D. V. Jahagirdar, Himalaya Publishing House
- 4) General Chemistry Experiments, Anil. J Elias, University press (2002)
- 5) Ligand Field Theory, B. N. Figgis.

## **CHO-247: Organic Chemistry Practical**

(6 Credits)

## Use of chemistry software like MOPAC, ISIS draw, Chem office (Minimum 3 experiments) Purification techniques (any 5)

Purification of solvents and reagents using techniques like crystallization, distillation, steam distillation, vacuum distillation, drying and storage of solvents, sublimation etc.

- a) Chromatography: TLC, Column.
- b) Solvent extraction using soxhlet extractor

## 1. Three component mixture separation and analysis using ether. (8 mixtures minimum including amino acid)

#### 2. Single stage preparations (minimum 9 preparations)

- a) 2-Methoxy naphthalene to 1-formyl-2- methoxy naphthalene
- b) Toluene to 4-methyl acetophenone
- c) Anthranilic acid to 2-iodo /2-choro benzoic acid
- d) Cyclohexanol to cyclohexanone
- e) Benzophenone to diphenyl methane
- f) Benzyl cyanide to phenyl acetic acid
- g) Benzaldehyde to chalcone
- h) Gycine to Benzoylglycine
- i) Nitrobenzene to m-di-nitrobenzene
- i) m-di-nitrobenzene to m-nitroaniline
- k) Benzoic acid to ethylbenzoate
- 1) Diel's Alder reaction of anthracene and maleic anhydride
- m) Chlorobenzene to 2,4-dintro chlorobenzene

#### Reference books

n) 1. Textbook of practical organic chemistry – A.I. Vogel

## M.Sc. Drug Chemistry

## **Practical**

#### CHD-128: INORGANIC AND ANALYTICAL CHEMISTRY PRACTICALS

(6 Credits)

- 1. Inorganic synthesis and characterization by physical or chemical methods:
  - a) Cis-trans potassium diaquo dioxalate chromate (III)
  - b) Chloropentammino cobalt (III) chloride.
- 2. Colorimetry;

Keg of M-L systems such as:

- i) Fe (III) Salicylic acid
- ii) Fe (III) Sulphosalicylic acid
- iii) Fe (III) resorcilic acid by Job's method and Mole ratio method
- 3. Photometric titration of systems such as:
  - a)  $Cu^{2+}$  EDTA
  - b) Fe<sup>2+</sup> Sulphosalicylic acid
  - c) Co<sup>2+</sup> R-nitroso salt.
- 4. Potentiometry:
  - a) Complexometric determination using disodium EDTA of
  - i) Co<sup>2+</sup>
  - jj) Al<sup>3+</sup>
  - iii) Cu<sup>2+</sup>
- 5 Solvent extraction of Al / Mo usmg 8-hydroxy quinoline complex and determination by spectrophotometry
- 6. Solvent extraction of ferric thiocyanate complex and determination by colorimetry.
- 7. Separation and estimation of Fe and Al on a cation exchanger.
- 8. Separation and estimation of copper and cobalt on cellulose column.
- 9. Analysis of Vitamin C in juices and squashes.
- 10. Analysis of Vitamin A in food products.
- 11. Simultaneous determination by titanium and vanadium Pt and Pd using hydrogen peroxide by spectrophotometry.

- 12, Estimation of Na, K and Ca in binary mixture by flame photometry using Li as Internal standard and using standard addition method.
- 13. Determination of the strength of the following by fiourimetmy, beryllium, aluminium, vitamin B1, vitamin B2.
- 14. Determination of the strength of commercial phosphoric acid/vinegar by conductometric titration.
- 15. Analysis of malathion by colorimetry or polarography.
- 16. Estimation of nitrile, fluoride, dissolved chlorine, chloride, iron, chromium, manganese colorimetrically.
- 17. Estimation of Hg, Pb, Cd spectrophotometrically/complexometrically.
- 18. Estimation of sulphadizine.
- 19. Estimation of mixtures of benzoic acid and salicylic acid in pharmaceutical preparations
- 20. Determination of iron, calcium and phosphorous in milk powder.
- 21. Partition coefficient.

#### References:

- 1) A textbook of Qualitative Inorganic Analysis3<sup>rd</sup> Edn., A. I Vogel, ELBS.
- 2) A Textbook of Practical Organic Chemistry, 4<sup>th</sup> Edn., A. I. Vogel, ELBS.
- 3) Standard Methods of Chemical Analysis, 6<sup>th</sup> Edn.; A series of volumes edited by F. J. Weicher, Robert E. Krieger Publishing co.
- 4) Pharmacoepoeia of India.

# CHD-108: Practical Course in Separation, Purification & Analytical techniques in Drug Chemistry (5 Credits)

- 1. Purification of solvents and reagents
- 2. Mixture separation Two and Three components.
- 3. Isolation of Natural products from Clove, Cinnamom by steam distillation. Also use Soxhlet apparatus for one natural product.
- 4. Chromatographic techniques as TLC, Coloumn chromatography
- 5. Biomolecule separation and identification using Gel Electrophoresis, Paper chromatography Immunoelectrophoresis.

- 6. Separation and Identification of active drug ingredients from commercial pharmaceutical preparations.
- 7. Try to use spectral data whenever possible.
- 8. Any current techniques as per need and demand.

#### **CHD-248: ORGANIC CHEMISTRY PRACTICALS**

(5 Credits)

- 1. Techniques: Crystallization, fractional crystallisation, fractional distillation, vacuum distillation, sublimation, steam distillation.
- 2. Single stage preparation involving different type of reactions (minimum 8 preparations).
- 3. Two-stage preparations (minim 2 preparation).
- 4. Three-stage preparations (minimum 2 preparations).
- 5. Derivatives of functional groups such as acetyl, benzoyl, 2, 4-DNP, oxime, anilide, amide and aryloxy acetic acid (minimum one of each type)

Typical preparations from which the single and two stage preparations can be chosen are:

- 1. Toluene p-nitrotoluene p-nitrobenzoic acid p-amino benzoic acid
- 2. Benzene Acetopheneone Acetophenone oxime Acetanilide
- 3. Benzaldehyde Benzoin Benzil Benzillic acid
- 4. Nitrobenzene m-dinitrobenzene m-nitroaniline m-nitrophenol
- 5. Phthalic acid phthalic anhydride phthalimide Anthranilic acid
- 6. Anthranilic acid pheylglycine orthocarboxylic acid indigo
- 7. Acetophenone Benzalacetophenone epoxide
- 8. Cyclohexanone Cyclohexanone oxime—caprolactam
- 9. Phthalic anhydride—o-benzolylbenzoic acid—anthraquinone.
- 10. O-Cholobenzoinc acid —N-phenylanthranilic acid —acridone.
- 11. Cholrobenzene—2,4-dinitrochlorobenzene —2,4-dinitrophenol
- 12. Bromobenzene—triphenylcarbinol-tritylchloride
- 13 Resorcinol—resacetophenone 4-ethyl resorcinol
- 14. Phenol—allylphenyl ether—o-allylphenol
- 15. Phenol —salicylaldehyde—coumarin