

**DEPARTMENT OF CHEMISTRY  
UNIVERSITY OF DHAKA  
DHAKA**



**CURRICULUM FOR  
M.S. IN CHEMISTRY**

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**DEPARTMENT OF CHEMISTRY**  
**UNIVERSITY OF DHAKA**

**M.S. Program in Chemistry**

The **Guidelines for Letter Grading System for M.S. Program in Chemistry** for the Department of Chemistry under the Faculty of Science.

**1. The M.S. Degree Program in Chemistry**

The M.S. degree program in the Department of Chemistry under the faculty of Sciences, University of Dhaka is of one academic year. Four different M.S. degrees are offered by the Department of Chemistry. These are (i) M.S. in Physical Chemistry (thesis group), (ii) M.S. in Organic Chemistry (thesis group), (iii) M.S. in Inorganic and Analytical Chemistry (thesis group) and (iv) M.S. in Chemistry (non-thesis group). A student can enroll either in Thesis Group or in Non-thesis Group where applicable.

The distribution of credits for Thesis and Non-Thesis students will be according to the following format.

Thesis Group		Non-Thesis	
Theory 3 credits $\times$ 6	18 credits	Theory 3 credits $\times$ 7	21 credits
Thesis	10 credits	Practical course 3 credits $\times$ 3	9 credits
General viva	2 credits	General viva	2 credits
Oral on thesis	2 credits	<b>Total</b>	<b>32 credits</b>
<b>Total</b>	<b>32 credits</b>		

**2. Admission into M.S. Courses**

Students who have completed B.S. (Hons.) degree from the Department of Chemistry, University of Dhaka with minimum CGPA of 2.5 in the scale of 4 will only be eligible for admission to M.S. courses in the Department of Chemistry under the Faculty of Science, University of Dhaka.

**3. Distribution of the Duration of the Program**

The duration of M.S. program will be distributed as follows over 1 (one) academic year.

24 weeks	For holding classes
04 weeks	Preparation for final examinations
04 weeks	Course final examination
16 weeks	Submission of thesis /projects /practical /examination/ seminar/internship
04 weeks	Publication of results

#### 4. Evaluation Procedure

The performances of the students will be evaluated on the basis of continuous assessment and course final examination. The marks in a course will be distributed as follows:

(a) **Theory Course**

Class Attendance	05%
In-course assessment / tutorial / assignment	25%
Course final examination	70%

(b) **Practical Course**

Class attendance	05%
Continuous assessment during Lab (non-thesis)	35%
Course final examination	60%

(c) **Marks for Attendance**

<b>Attendance (%)</b>	<b>Marks (%)</b>
90 and above	05
85 to 89	04
80 to 84	03
75 to 79	02
60 to 74	01

#### 5. In-course Assessment (Theory Courses)

- (i) The course teacher will announce the dates of in-course examinations at the beginning of the course. The in-course assessment will be based on tests/assignments/seminars or class-presentations. The number and distribution of tests/assignments/seminars/class-presentations or any combination of them will be decided by the respective course teacher. The in-course test will be of one hour duration and the teacher concerned will be responsible to assess the students sitting in his/her course. There will be 2 tests for a 3 credit course and average of the two should be considered to finalize the grade.

**Answer scripts must be shown to the students.**

- (ii) No make-up test will be arranged for a student who fails to appear or wish to re-appear in his/her in-course test/tests. Absence in any in-course test will be counted as zero for calculating the average in in-course test for that course. However, a student can request special permission for re-take of in-course test if recommended by the course teacher through the academic committee of the Department only under extraordinary circumstances (e.g., accident, death of a close-relative, etc.).

## **6. Eligibility for Sitting in Course Final Examination**

- (i) A student must attend **at least 75%** of the total classes in a course held in an academic year to be eligible for appearing in the final examination.
- (ii) A student attending at least 60% of classes in a course will be allowed to sit for course final examination after payment of non-collegiate fees as decided by the University.
- (iii) A student attending less than 60% classes in a course will not be allowed to sit for final examination.

## **7. Course Final Examination**

- (i) An Examination Committee consisting of three (3) internal members and one (1) external member will be formed.
- (ii) The course final examination will be conducted by the Controller of Examinations as per existing rules of the University.
- (iii) There will be two examiners working as question setters and answer-script evaluators. One of them must be the course teacher and the external examiner will preferably be from outside the respective Department. In case a suitable person is not available as external examiner a teacher from within the Department may be appointed with prior permission from the Vice Chancellor.
- (iv) The course final examination will be of 3 hours for 3 credit course.
- (v) Examination of practical courses for non-thesis students will be conducted as per existing rules of the University.
- (vi) A course viva voce examination will be conducted by the Examination Committee members immediately after completion of the examination of theoretical and laboratory courses for both thesis groups and non-thesis group students.
- (vii) Thesis students must submit their thesis within 16 weeks from the date of last examination.
- (viii) After submission of the thesis, students will appear in oral defense of their thesis before the Examination Committee. Supervisor of a student will be requested to be present at the time of the presentation. He/she may participate in discussion but not in evaluation.

## **8. Evaluation of Thesis**

Thesis will be evaluated as per existing rules of the University with two external examiners from outside the respective Department.

## 9. The Grading System

Marks obtained by a student in different courses will be converted to grades. A basic four point (4.00) grading scale will be followed. The following letter grade and grade point will be used to determine the student's grade point average (GPA).

Marks Obtained	Corresponding Letter Grade	Grade Point
80% or above	A+	4.00
75 to 79%	A	3.75
70 to 74%	A-	3.50
65 to 69%	B+	3.25
60 to 64%	B	3.00
55 to 59%	B-	2.75
50 to 54%	C+	2.50
45 to 59%	C	2.25
40 to less than 44%	D	2.00
Less than 40%	F	0.00

## 10. Improvement

- (i) If a student obtains a grade C+ or lower in a theory course he/she will be allowed to repeat the term-final examination only once with the following batch for the purpose of grade improvement, but he/she will not be eligible to get a grade better than 'B+' in such a course. A student failing to improve his/her grade in a course can retain the earlier grade.
- (ii) A student will be allowed to take improvement of 25% of the total theoretical credits taken.
- (iii) A student obtaining 'F' grade in one or more courses (theory and practical) will not be awarded degree. However, a student obtaining 'F' grade in a course may be allowed to retake that course only once with the next batch of students in order to be awarded a degree. A student obtaining 'F' grades in more than one course will not be allowed to repeat any course.

## 11. Calculation of GPA

The GPA (grade point average) will be calculated according to the following formula:

$$\text{GPA} = \frac{\sum(\text{Grade points in a course} \times \text{Credits for the course})}{\text{Total credits taken}}$$

## **12. Credits Required for Degree**

A student must earn GPA 2.5 on a scale of 4.00 with 32 credits to complete the requirements for the award of M.S. degree in the different branches of chemistry.

## **13. Readmission**

- (i) A student failing to complete the M.S. course in a year may seek readmission with the next available batch of students, provided he/she applies within one month of publication of the result of the concerned year.
- (ii) A readmitted student will be allowed to retain his/her in-course/class assessment/tutorial marks earned in previous year.
- (iii) A readmitted student may be allowed to take up thesis work as decided by the Departmental Academic Committee.
- (iv) The transcripts of successful readmitted student will bear the letter 'R' after GPA with a foot note explaining 'R' means Readmission.

## **14. General Regulations**

- (i) The Departmental Academic Committee will design courses of studies, frame syllabuses of different courses, propose examination committee and panel of examiners as per rules of the University.
- (ii) The course teacher will provide the students a course outline, schedule of class assessment and relevant information in the first class of the term.
- (iii) The course teacher shall announce the results of the in-course tests within four weeks of the date of holding the tests and submit the marks to the Chairman of the Examination Committee for the respective batch and also a copy to the Controller of Examinations at least two weeks before the start of the final examination. He/she should also submit a statement showing the total number of classes held and the percentage of attendance of each student in his/her course to the Chairman of the Department.
- (iv) Tabulation work will be started only after all the marks of the course final examinations for the year are received by the Chairman of the Examination Committee. Marks received by the Chairman of the Examination Committee shall remain in the sealed envelope as sent by the Examiner/Examiners until tabulation work is started.
- (v) The present system of conducting course final examination and publication of results by the office of the Controller of Examinations shall continue.
- (vi) For any other matters not covered in these rules, the existing rules of the University of Dhaka will be applicable.

### **Outline of Syllabus for M.S. (Thesis Group) in Physical Chemistry**

Course No.	Course Title	Credits
PC 501	Advanced Chemical Kinetics	3
PC 502	Advanced Surfaces Chemistry and Catalysis	3
PC 503	Advanced Photochemistry	3
PC 504	Advanced Electrochemistry and Electrochemical Techniques	3
PC 505	Biophysical Chemistry	3
PC 506	Chemistry of the Atmospheric Environment	3
PC 507	Molecular Symmetry and Advanced Spectroscopy	3
PC 508	Supramolecular and Nanochemistry	3
PC 509	Chemistry of Materials	3
PC 510	Advanced Concepts of Liquids	3
PC 511	Advanced Polymer Chemistry	3
PC 512	Computational Chemistry	3

Course No. PC 503 and PC 507 are compulsory courses. Students will take 4 other courses from the rest.

### **Outline of Syllabus for M.S. (Thesis Group) in Organic Chemistry**

Course No.	Course Title	Credits
ORG 521	Advanced Reaction Mechanism	3
ORG 522	Advanced Stereochemistry	3
ORG 523	Spectroscopic Methods in Organic Chemistry	3
ORG 524	Separation and Chromatographic Techniques	3
ORG 525	Organic Synthesis	3
ORG 526	Carbohydrates and Glycoconjugates	3
ORG 527	Natural Products	3
ORG 528	Advanced Heterocyclic Compounds and Caged Hydrocarbons	3
ORG 529	Organic Pollutants in the Environment	3
ORG 530	Advanced Medicinal and Pharmaceutical Chemistry	3
ORG 531	Food Chemistry and Technology	3

Course No. ORG 521 and ORG 523 are compulsory courses. Students will take 4 other courses from the rest.

## Outline of Syllabus for M.S. (Thesis Group) in Inorganic and Analytical Chemistry

Course No.	Course Title	Credits
IA 541	Advanced Coordination Chemistry	3
IA 542	Organometallic Chemistry	3
IA 543	Bioinorganic Chemistry	3
IA 544	Inorganic Polymers and Macromolecules	3
IA 545	Nuclear and Radiochemistry	3
IA 546	Material Science	3
IA 547	Solution Chemistry	3
IA 548	Advanced Chemical Crystallography	3
IA 549	Instrumental Methods of Chemical Analysis	3
IA 550	Electroanalytical Chemistry	3
IA 551	Environmental Monitoring and Analysis	3
IA 552	Chemistry of Aquatic and Biotic Environment	3

Course No. IA 541 and IA 549 are compulsory courses. Students will take 4 other courses from the rest.

## Outline of Syllabus for M.S. (General Group) in Chemistry

### 1. Theory Compulsory Courses

Course No.	Course Title	Credits
PC 503	Advanced Photochemistry	3
PC 507	Molecular Symmetry and Advanced Spectroscopy	3
ORG 521	Advanced Reaction Mechanism	3
ORG 523	Spectroscopic Methods in Organic Chemistry	3
IA 541	Advanced Coordination Chemistry	3
IA 549	Instrumental Methods of Chemical Analysis	3

### 2. Theory Optional Course

Students will have to take one more course from the remaining courses from three different branches of chemistry.

### 3. Laboratory Courses

Three (3) compulsory laboratory courses are as

PC 515	Physical and Environmental Chemistry Laboratory
ORG 535	Organic Chemistry Laboratory
IA 555	Inorganic and Analytical Chemistry Laboratory

## Detailed Syllabus for M.S. (Thesis Group) in Physical Chemistry

### PC 501 Advanced Chemical Kinetics

(3 Credits)

#### Learning Objectives

The learning objectives of this course are to

- (i) Provide advanced concept of chemical kinetics of different elementary and composite reactions, micellar catalysis and reactions in nano systems.
- (ii) Impart knowledge on steady state approximation and its applications, and theories of reaction rates.
- (iii) Give the idea about potential energy surface (PES), contour diagram, ion-dipole and dipole-dipole reactions, theory of diffusion controlled reactions.
- (iv) Provide concepts on Hammett equation, kinetics of fast reactions and their applications.
- (v) Give knowledge about molecular dynamic calculations and state to state kinetics.

#### Course Content

1. **Composite Reactions:** Composite reactions, concept of steady state approximation and steady state treatment, rate equations for composite reactions: decomposition of ozone, hydrocarbon oxidation and combustion of hydrocarbons, oscillation reaction, Belousov-Zhabotinski (B-Z) reaction, a schematic representation of the B-Z reaction, chemistry of B-Z reaction, stationary flames, thermal explosion, isothermal explosion, branching chain explosion, hydrogen oxygen reaction, explosion limits. Oscillatory reaction.
2. **Theories of Reaction Rates:** Review of theories: Collision theory and conventional transition state theory (CTST). relationship between critical energy and activation energy, probability factor, limitations of collision theory, limitations of the conventional TST, thermodynamic treatment of the TST, statistical treatment of TST, contour diagram, potential energy surface (PES), some applications of the CTST, reactions between atoms and molecules, reaction between H and HBr.
3. **Reactions in Solutions:** Review of reactions in solutions. The Bronsted relation, linear free energy relations, ion-dipole and dipole-dipole reactions, theory of diffusion-controlled reactions, full microscopic and partial microscopic diffusion-controlled reactions, diffusion control in ionic reactions, substituent and correlation effects, Hammett equation and its applications.
4. **Kinetics of Fast Reactions:** Flow techniques, plug and stirred flow method, stopped flow and continuous flow methods, contact time,

relaxation methods, temperature jump and pressure jump, flash photolysis, light sources for flash photolysis, detection techniques for flash photolysis experiments, absorption spectroscopy, fluorescence techniques, resonance fluorescence, LASER induced fluorescence and relative methods.

5. **Micellar Catalysis:** General features of micellar catalysis, aqueous micelles as models for enzymatic interactions, micellar catalysis of hydrolyses, solvolyses and aminolyses, micellar effects on ionic reactions, catalysis by reverse micelles in non-aqueous solvents and microemulsions, catalysis in liquid crystalline and ternary systems, general mechanisms of micellar catalysis: kinetic models.
6. **Kinetics of Chemical Reactions in Nanosystems:** Stochastic approach, diffusion controlled reaction in nanosystems. Reactions inside the sphere, mean reaction time approximation, reactions on the surfaces of the nanospheres. Decay kinetics of nanosystems, rate constant concept for reactions in nanosystems, Fractal approach to kinetics in restricted systems.
7. **Reaction Dynamics:** Molecular dynamical calculations- the reaction  $H + H_2$ , the reaction  $Br + H_2$ . Potential energy surfaces, attractive, repulsive, and intermediate type surfaces for exothermic reactions, selective enhancement of reactions, disposal of excess energy, gradual and sudden surface influence of rotational energy. Molecular beams, stripping and rebound mechanisms, state-to-state kinetics.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand the advanced concepts on chemical kinetics of different types of chemical reactions.
- (ii) Discuss different theories of reaction rates and apply statistical and thermodynamic treatment of TST.
- (iii) Demonstrate knowledge on Hammett equation, kinetics of fast reactions and their applications.
- (iv) Describe the kinetics of chemical reactions in nano-system including micellar catalysis.
- (v) Explain state to state kinetics, attractive and repulsive surfaces, molecular dynamical calculations for the reactions between atoms and molecules.

### Books Recommended

1. Chemical Kinetics, K. J. Laidler.
2. Kinetics and Mechanism, A. A. Frost and R. G. Pearson.
3. Concepts of Modern Catalysis and Kinetics, I. Chorkendorff and J. W. Niemantsverdriet.

4. Catalysis in Micellar and Macromolecular Systems, J. H. Fendler and E. J. Fendler.
5. Micellar Catalysis, Surfactant Science Series, Volume 133, M. N. Khan.
6. Introduction of Nanoscience, S. M. Lindsay.

## **PC 502 Advanced Surface Chemistry and Catalysis (3 Credits)**

### **Learning Objectives**

The learning objectives of this course are to

- (i) Give modern concepts on physicochemical characteristics of solid surfaces, adsorption and energetic involved.
- (ii) Impart advanced knowledge on catalysis and preparation, characterization and industrial applications of catalysts.
- (iii) Aware on adsorption thermodynamics, kinetics of catalytic reactions and their mechanism.
- (iv) Give idea on basic principle, operation and applications of different modern techniques for characterization of solid surfaces.

### **Course Content**

1. **Properties of Solid Surface:** Physical properties of solid surface: pore structure, pore volume distribution, void volume and solid density, surface area, determination of surface area. Electrical properties of solid surface: surface electron potential, surface space charge, surface free energy. Structures of metals and metallic oxides, surface structure and stepped planes. Surface modification: coatings, crack formation and propagation.
2. **Adsorption Energetics:** Physisorption and chemisorption, isotherms, isobars, enthalpy and entropy changes. Trends in surface reactivity: one dimensional model of energetics of physisorption and chemisorption. Work function, work function change due to adsorption, spontaneous self-organization.
3. **Surface Reactions Kinetics:** Elementary surface reaction, adsorption and sticking, determination of sticking coefficient, Lagergren pseudo-first order and pseudo-second order equation, intra-particle diffusion model, Elovich equation, Langmuir isotherms for associative, dissociative and competitive adsorption. Langmuir-Hinshelwood and Eley-Rideal mechanism kinetics, micro-kinetic modeling.
4. **Mechanism of Surface Reactions:** General considerations in the determination surface reaction mechanism, adsorption sites, orientation of adsorbate, adsorbate induced reconstruction, lateral interactions in surface reactions, intermediates in surface reactions, transition state

theory of surface reactions, reaction pathway of catalyzed and noncatalyzed reaction, Tempkin equation, surface diffusion of adsorbed species, geometry of adsorbate and adsorbent after chemisorption, mechanism of chemisorption process on solid surface. Desorption, activation energy of desorption, temperature programmed desorption studies.

5. **Catalysis:** General description of catalyst, catalyst preparation, metallic catalyst, supported metal catalyst, non-metallic catalyst, metal oxide, mixed metal oxide, zeolite and bio-catalysts. Modification of catalyst, catalyst deactivation, turnover number, specificity and selectivity in catalysis, catalytic activity, catalysis by transition metals: hydrogenation, dehydrogenation, hydrogenolysis, the volcano curve, catalytic oxidation of CO and  $\text{NH}_3$  on metal and metal oxide surfaces, oxidation on oxide surfaces, hydrocarbon conversion, reforming catalysts.
6. **Solid Catalysts in Environmental and Industrial Processes:** Automotive exhaust catalysis, three way catalyst, catalytic reactions in three-way catalyst, selective catalytic reduction. Hydrogenation of vegetable oils, ammonia and nitric acid production, synthesis gas conversion, ethylene oxide production, sulphuric acid production, linear polyethylene production, catalytic cracking, synthetic gasoline production.
7. **Techniques for Characterization of Solid Surfaces and Adsorbed Species:** Electron emission spectroscopy: ultraviolet photoelectron spectroscopy (UPS), X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES) and extended X-ray absorption fine structure spectroscopy (EXAFS), electron energy loss spectroscopy (EELS), low energy electron diffraction (LEED). Electron microscopy: scanning electron microscopy (SEM), transmission electron microscopy (TEM), scanning tunneling microscopy (STM), atomic force microscopy (AFM), field emission microscopy (FEM), field ion microscopy (FIM), surface enhance Raman spectroscopy (SERS) and reflectance spectroscopy.

## Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand the physicochemical characteristics of solid surfaces.
- (ii) Know the methods of preparation, characterization and industrial applications of catalysts.
- (iii) Demonstrate knowledge on adsorption thermodynamics, kinetics of catalytic reactions and their mechanism.
- (iv) Apply knowledge on basic principle, operation and applications of different modern techniques for characterization of solid surfaces.

## Books Recommended

1. Physical Chemistry of Surfaces, A. W. Adamson and A. P. Gast.
2. Atkin's Physical Chemistry, P. W. Atkins and J. W. Paula.
3. Surface Chemistry, E. M. McCash.
4. An Introduction to Chemisorption and Catalysis by Metals, Von R. P. H. Gasser.
5. Concepts of Modern Catalysis and Kinetics, I. Chorkendoff and J. W. Niemantsverdriet.
6. Introduction to Surface Chemistry and Catalysis, G. A. Somorjai.
7. Surface Science: Foundations of Catalysis and Nanoscience, K. W. Kolasinski.
8. Internal Reflection and ATR Spectroscopy, M. Milosevic.
9. Selected Articles from Recent Journals.

## PC 503 Advanced Photochemistry

(3 Credits)

### Learning Objectives

The learning objectives of this course are to

- (i) Give general concepts on photochemical and radiochemical processes and use of various light sources in photochemistry.
- (ii) Impart knowledge on different photophysical and photochemical processes and related terminologies.
- (iii) Demonstrate a detailed knowledge on photoactive materials and their applications; such as photoelectrochemical solar cells, photovoltaic cells etc.
- (iv) Give knowledge on different advanced oxidation processes for treatment of water and photodegradation of dyes and other organic substances.
- (v) Introduce different advanced techniques for study of photochemical behavior; such as flash photolysis, matrix isolation etc.

### Course Content

1. **General Consideration:** Pathways of dark reactions and photochemical reactions. Photochemistry and radiation chemistry. Dosimeters. Current trends in photochemistry.
2. **Light Sources in Photochemistry:** Solar energy and solar simulation, Filament lamp, Discharge lamp, Lasers: basic principle of laser action; various types of lasers. Characteristics of laser radiation, Continuous and pulsed laser. Determination of light intensity. Actinometry.
3. **Photophysical and Photochemical Processes:** Excited species and their fates. Jablonski diagram. Non-radiative and radiative processes. Fluorescence. Factors contributing to fluorescence. Delayed

fluorescence. P-type and E-type delayed fluorescences. Phosphorescence. Kinetics of photophysical processes. Unimolecular and bimolecular processes. Photochemical quenching. Stern-Volmer equation. Excimers. Exciplexes. Intermolecular electronic energy transfers: Radiative mechanism. Long range dipole-dipole energy transfer. Short range electron exchange energy transfer (photosensitization). Kinetics of some photochemical reactions. Photochemical processes in atmosphere. Photochemical formation and degradation of ozone. Photochemistry of troposphere. Photochemistry of metal complexes. Ligand exchange. Redox processes. Photolysis of anthracene in an inert solvent. Photochemistry of alkenes. Photochemistry of carbonyl compounds. Chemiluminescence and Bioluminescence.

4. **Photoactive Materials and Their Applications:** Semiconducting metal oxides and their photochemistry. Types of photoelectrochemical solar cells. Solar energy conversion by photovoltaic cells. Dye sensitized photovoltaic cells. Semiconductor sensitized water splitting. Semiconductor mediated photocatalysis. Organic solar cells. Storage of solar energy. Mechanism of energy conversion. Energy conversion efficiency.
5. **Advanced Oxidation Processes (AOP's) in Water Treatment:** Types of AOP's. The hydrogen peroxide/ultraviolet light ( $\text{H}_2\text{O}_2/\text{UV}$ ), ozone/ultraviolet light ( $\text{O}_3/\text{UV}$ ), hydrogen peroxide/Ozone ( $\text{H}_2\text{O}_2/\text{O}_3$ ), hydrogen peroxide/ultraviolet light/ozone ( $\text{H}_2\text{O}_2/\text{O}_3/\text{UV}$ ),  $\text{TiO}_2$  or  $\text{ZnO}/\text{UV}$  and  $\text{TiO}_2$  or  $\text{ZnO}/\text{UV} + \text{H}_2\text{O}_2$  processes.
6. **Photodegradation:** Degradation of dyes and other organic substances in aqueous system. Roles of mediators, hydrogen peroxide and ozone. Influence of light on TOC and BOD of the dye house effluents in the presence of photocatalysts and other agents. Kinetics of photodegradation of dyes in aqueous solution.
7. **Techniques in Photochemistry:** Fluorescence spectroscopy. Phosphorescence spectroscopy. Flash photolysis techniques in photochemistry: Pico- and Femtosecond photolysis. Flash photolysis studies of bimolecular electron transfer and other photochemical reactions. Time resolved IR spectroscopy. Detection of short-lived species: Matrix isolation. Laser induced breakdown spectroscopy (LIBS).

## Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand the differences between dark and photochemical reactions; realize the principle and application of different light sources.

- (ii) Describe different photophysical and photochemical processes and detailed on fluorescence, phosphorescence and related phenomena.
- (iii) Realise photoactive materials and their applications; such as photoelectrochemical solar cells, photovoltaic cells etc.
- (iv) Apply knowledge of different advanced oxidation processes for treatment of water and photodegradation of dyes and other organic substances.
- (v) Use different advanced techniques for study of photochemical behavior; such as flash photolysis, matrix isolation etc.

### **Books Recommended**

1. Photochemistry, J. G. Culvert and J. N. Atkins.
2. Principles and Application of Photochemistry, B. Wardle.
3. Principles of Molecular Photochemistry. An Introduction, N. J. Turro, V. Ramamurthy and J. C. Scaiano.
4. Principles and applications of Photochemistry, R. P. Wayne.
5. Fundamentals of Photochemistry, K. K. Rohatgi - Mukharjee.
6. Principles of Radiation Chemistry, J. H. O' Donnel and D. F. Sangster.
7. Selected Articles from Recent Journals.

## **PC 504 Advanced Electrochemistry and Electroanalytical Techniques (3 Credits)**

### **Learning Objectives**

The learning objectives of this course are to

- (i) Explain the mechanism of formation of electrical double layer and their models.
- (ii) Provide knowledge on advanced dynamic and static voltammetric techniques and their comparison with classical polarographic techniques.
- (iii) Impart knowledge on development of analytical methodology, various electrode mechanisms, kinetic and mass transport processes.
- (iv) Explain electrode surface morphology using spectroscopic and microscopic techniques.

### **Course Content**

1. **Electrified Interface and Electrode:** Formation of electrified interfaces. Electrical double layer and different models. Butler-Volmer equation and its modifications and applications. Thermodynamic treatment of the equilibrium state for charge transfer at the metal/solution interface. Mass transport and electrode processes: Faradaic and non-Faradaic processes, Nernst-Planck equation, Nernstian and non-Nernstian behaviour, Fick's first and second law and its application in mass transport, kinetic and transport controlled processes.

2. **Sweep Voltammetry:** Linear and cyclic voltammetry: principles, switching potential and potential excitation signal, generation of cyclic voltammogram from concentration-distance profiles. Diagnosis of reversible, quasi-reversible, irreversible charge transfer and coupled chemical kinetics from cyclic voltammetry. Cyclic voltammetry at microelectrodes. Applications of linear and cyclic voltammetry.
3. **Step Techniques:** Basic principles, potential excitation signals and response signals of chronoamperometry, chronocoulometry and chronopotentiometry (single and double potential steps). Use of Cottrell and Sand equations and applications. Evaluation of heterogeneous kinetic parameters and charge for adsorption.
4. **Pulse and Stripping Techniques:** Pulse techniques: fast, normal & differential pulse and square wave voltammetry (principle, comparative potential excitation signals and response signals), pulse width diminution factor. Application and relative advantages of different pulse techniques. Some special pulse techniques: reverse pulse, differential normal pulse and double differential pulse voltammetry. Stripping techniques: different types of stripping techniques (anodic, cathodic, potentiometric, adsorptive and abrasive), and their comparative pre-concentration and determination step. Use of pre-concentration techniques at trace and ultra-trace level analysis. Use of pre-concentration step for mercury film electrode and its use in metal-ligand complex study (de Ford and Hume method).
5. **Hydrodynamic Voltammetry:** Useful parameters (comparison of diffusion layer thickness: dynamic and static condition, relation of hydrodynamic condition with Reynolds, Schmidt, Peclet and Sherwood numbers). Practical considerations (Potentiostat and electrodes in hydrodynamic system: RDE and RRDE). Reversible and irreversible kinetics in hydrodynamic condition. Use of Levich, Koutecky-Levich equations and Tafel plot and applications. Evaluation of kinetic control and diffusion control processes. Applications of hydrodynamic voltammetry.
6. **Impedance Techniques:** General of Impedance. Detection and measurements of Impedance. Equivalent circuit of an electrochemical cell. The Faradaic Impedance of a simple electrode process The Faradaic impedance,  $Z_f$ , and the total impedance. Impedance plots for complex plane. Admittance and its use. Hydrodynamic electrodes and impedance. Transforms and impedance, application of impedance for characterization corrosion and capacitors.
7. **Electrochemical Quartz Crystal Microbalance, Spectro-electrochemistry and Scanning Electrochemical Microscopy:** principles, electrochemical set-up and applications, electro-

chemiluminescence, optical probing of electrode-solution interfaces. Approach curves for scanning electrochemical microscopy, imaging surface topography, applications in homogeneous reaction kinetics and others.

### **Learning Outcomes**

Upon completion of this course, the students will be able to

- (i) Explain the formation, mechanism and different models of electrified interfaces.
- (ii) Gain knowledge on development of some advanced static and dynamic electrochemical techniques.
- (iii) Apply knowledge of static and dynamic electrochemical techniques in various applications such as development of electroanalytical techniques, metal-ligand complexation study, corrosion protection etc.

### **Books Recommended**

1. Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology and Environmental Science, J. O'M. Bockris and A. K. N. Reddy.
2. Electrochemistry, Principles, Methods and Applications, C. M. A. Brett and A. M. O. Brett.
3. Electroanalytical Chemistry, J. Wang.
4. Electrochemical Methods, Principles and Applications, A. J. Bard and L. R. Faulkner.
5. Laboratory Techniques in Electroanalytical Chemistry, P. Kissinger and W. R. Heineman.

## **PC 505 Biophysical Chemistry**

**(3 Credits)**

### **Learning Objectives**

The learning objectives of this course are to

- (i) Deal with enzyme kinetics, cooperative binding, allosteric interactions in biological system.
- (ii) Compare thermodynamics and standard states of physical science with those of biological system, and understand bioenergetics involving ATP, glycolysis, Krebs cycle etc.
- (iii) Describe biological membrane, models for studying membrane, diffusion through membrane, Donnan effect.
- (iv) Deals with design and application of biosensors.
- (v) Understand the structure of protein (macromolecules), ligand-macromolecule binding equilibrium, solubility of proteins, dissociation of amino acids, biological buffer, etc.

## Course Content

- 1. Enzyme Kinetics:** Introduction to enzyme, characteristics, mechanisms, kinetic equations, enzyme-substrate interactions, multisubstrate systems, enzyme inhibition, effect of pH on enzyme kinetics. Cooperative binding, quantitative analysis of cooperative binding by Hill plot, oxygen binding of myoglobin and hemoglobin, factors influencing the oxygen binding, Bohr effect. Allosteric interactions, features and properties of allosteric enzymes, Monod-Wyman-Changeux (MWC) model, experimental tests of the MWC model, alternative models for allosteric proteins; a sequential model, a more general scheme.
- 2. Bioenergetics:** Introduction, bioenergetics and thermodynamics. Bioenergetics systems, mechanism of collection and utilization of energy in biological systems, coupling mechanism, phosphorylation, oxidative chain and substrate level phosphorylation. Self regulation of energy production, Biochemist's standard state, ATP-the carrier of energy, glycolysis, anaerobic and aerobic glycolysis, Krebs cycle, Limitations of thermodynamics.
- 3. Biological Membrane:** Structure and functions of biological membrane, diffusion through membrane- simple diffusion, facilitated diffusion, active transport,  $\text{Na}^+\text{-K}^+$  pump, co-transport. Membrane equilibria: general comments on equilibria across a membrane, osmotic pressure and pH difference across a membrane, Donnan effect, Donnan equilibria involving protein bearing single and multiple charges.
- 4. Models for Artificial Membrane and Cell:** Introduction, common lipids and their phase behavior, interactions of amino acid and protein with lipids. Models of biological membrane and cell; Langmuir monolayers, bilayers, vesicles or liposomes: structure and preparation of these models, conventional liposome formulations, targeted drug delivery using liposomes.
- 5. Biological Macromolecules:** Introduction, structure of proteins: primary, secondary, tertiary and quaternary structures, stability of protein conformation, factors responsible for stabilization, thermodynamic treatment of stability constant, protein binding, protein-ligand binding, binding equilibria, equilibrium dialysis, dynamic dialysis, hydrophobic interaction, denaturation of proteins, denaturing agents, mechanism of denaturation, protein binding and pharmacodynamics, complexation and drug action, metal complexation in biological systems, solubility of proteins: salting-in and salting-out effects.
- 6. Biosensors:** Introduction, types of sensors, micro-organism based sensor: glucose sensor, alcohol sensor, methane sensor, DNA sensors,

urea biosensor, BOD sensor etc., basic design of sensors, applications; food analysis, agriculture, environment, biomedical application.

- 7. Selected Topics in Biophysical Chemistry:** Dissociation of amino acids, isoelectric point, titration of proteins, buffer in biological systems, molecular recognition.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand the kinetics of enzyme catalysis and the factors affecting this kinetics.
- (ii) Explain the cooperative binding of oxygen with hemoglobin and myoglobin and the factors influencing this binding.
- (iii) Demonstrate the allosteric interaction of enzymes and the associated models developed for this interaction.
- (iv) Compare thermodynamics with bioenergetics and understand the ATP as energy carrier, glycolysis, Krebs cycle.
- (v) Understand the structure and function of biological membrane, membrane-ligand equilibrium,  $\text{Na}^+\text{-K}^+$  pump etc.

### Books Recommended

1. Physical Chemistry for the Biosciences, R. Chang.
2. Artificial Cells - Cell Engineering and Therapy, S. Prakash.
3. Biophysical Chemistry Part III: The Behaviour of Biological Macromolecules, C. R. Cantor and P. R. Schimmel.
4. Harper's Biochemistry, R. K. Murphy, D. K. Granner, P. A. Mayes and V. W. Rodwell.
5. Analytical Electrochemistry, J. Wang.
6. Biochemistry, A. Catarow and B. Schepartz.
7. Physical Pharmacy: Physical Chemical Principle in Pharmaceutical Sciences, A. Martin and J. Swarbrick.
8. Recent Publications in the Journals.

## **PC 506 Chemistry of the Atmospheric Environment (3 Credits)**

### Learning Objectives

The learning objectives of this course are to

- (i) Provide idea on primitive and present atmosphere, atmospheric chemistry, air pollution and toxic effects of various pollutants.
- (ii) Impart knowledge on monitoring of atmospheric pollutants and ongoing chemical processes in troposphere.
- (iii) Give details on ozone formation and depletion, ozone measurement, role of CFC on ozone depletion, ozone hole and international legislative initiatives.

- (iv) Impart knowledge on effect of various greenhouse gases in the troposphere and its effect on climate changes such as global warming.
- (v) Acquaint with the air quality standards and environmental regulations for air quality management.

## Course Content

1. **Atmosphere:** Origin and composition of atmosphere; earth atmosphere: its origin, composition, particles, aerosols, clouds; Cyclic processes: nitrogen, oxygen, water, carbon dioxide, sulphur, trace metal cycles, carbon cycles- link between biosphere and atmosphere; Structure of atmosphere: troposphere, stratosphere, mesosphere and ionosphere; Solar radiation; Radiative heating; Temperature profile; Inversion layer in the troposphere; Atmospheric transport and turbulence; Vertical transport; Winds; Effects of changes in atmospheric composition on climate.
2. **Air Pollution:** Criteria and non-criteria pollutants; Classification of air pollutants: primary and secondary pollutants; Regional and global air pollution; Regional air pollution: particulate, smog, acid rain; Toxic effects of various pollutants.
3. **Chemical Processes in the Troposphere:** Generation of reactive species: singlet and triplet oxygen atoms; Hydroxyl radicals; Nitrate radicals; The day-time chemistry; Formation of ozone and organic nitrates; The night-time chemistry; Wet and dry deposition of pollutants; Simulation studies in smog chambers.
4. **Monitoring of Atmospheric Pollutants:** Air sampling techniques; Spectrophotometric, chemical and gas chromatographic techniques for analysis of PM<sub>10</sub>, PM<sub>2.5</sub>, Soot Carbon, SO<sub>x</sub>, NO<sub>x</sub> and VOCs; Field sensors for CO, SO<sub>x</sub>, NO<sub>x</sub>, O<sub>3</sub> and hydrocarbons analysis.
5. **Stratospheric Ozone Depletion:** Ozone layer and stratospheric ozone; Chapman mechanism for the formation of ozone layer; Catalytic processes; Ozone depletion; Role of CFCs; Ozone depletion potential (ODP) of CFCs; UV spectrum of oxygen and ozone; Ozone measurement in the stratosphere: earth stations and satellite stations; Antarctic ozone hole, its detection and its formation; Impact of stratospheric ozone depletion; Legislative measures; HCFCs and their ODP. International legislative initiatives: Montreal protocol.
6. **Greenhouse Effect in the Troposphere and Its Impact on Climate Changes:** Various greenhouse gases, Sources and individual contribution of greenhouse gases; CO<sub>2</sub> and methane concentration in the atmosphere; Global warming and its impact on living system; GHG trading and clean technology; International legislative initiatives: Kyoto protocol.

## **7. Environmental Regulation for Air Quality Management: Air quality standards.**

### **Learning Outcomes**

Upon completion of this course, the students will be able to

- (i) Demonstrate knowledge on primitive and present atmosphere, atmospheric chemistry, air pollution and toxic effects of various pollutants.
- (ii) Monitor atmospheric pollutants and ongoing chemical processes in troposphere.
- (iii) Realize the ozone formation and depletion, ozone measurement, role of CFC on ozone depletion, ozone hole and international legislative initiatives.
- (iv) Demonstrate the effect of various greenhouse gases in the troposphere and its effect on climate changes such as global warming.
- (v) Gain concepts about the air quality standards and the available rules and regulations imposed for controlling the air pollution.

### **Books Recommended**

1. Chemistry of the Atmosphere, R. P. Wayne.
2. Atmospheric Chemistry and Physics from Air Pollution to Climate Change, J. H. Seinfeld and S. N. Pandis.
3. Introduction to Atmospheric Chemistry, D. J. Jacob.
4. Principles of Air Quality Management, R. D. Griffin.
5. Environmental Chemistry, S. E. Manahan.
6. Environmental Chemistry, A. K. De.
7. Environmental Hazards: Assessing Risk and Reducing Disaster, Keith Smith.
8. Air Monitoring by Spectroscopic Technique, M. W. Sigrist (Edited).

## **PC 507 Molecular Symmetry and Advanced Spectroscopy (3 Credits)**

### **Learning Objectives**

The learning objectives of this course are to

- (i) Achieve knowledge on molecular symmetry, group multiplication table, character table, the relation between molecular symmetry and infrared and Raman activities.
- (ii) Acquaint with advanced concepts of Raman and electronic spectroscopy.
- (iii) Give details on Mossbauer spectroscopy and its application.
- (iv) Achieve advanced knowledge on esr and nmr techniques, including details of  $^{13}\text{C}$  nmr and their interpretation.
- (v) Demonstrate skills and abilities needed for analysis of spectra.

## Course Content

- 1. Molecular Symmetry and Symmetry Groups:** Symmetry elements and symmetry operations; products of symmetry operations, the symmetry classification of molecules into point groups, classes of symmetry operations, Marci matrix representation of symmetry operation. Some immediate consequences of symmetry.
- 2. Group Theory and Its Application:** Definition and properties of a group. Group multiplication tables, representations of groups, properties of materials and vectors, reducible and irreducible representations. Great orthogonality theorem. Character tables and their uses; symmetry species of point groups. Distribution of fundamentals among the symmetry species. Vanishing integral and orbital overlap; vanishing integrals and selection rules for infrared and Raman activities.
- 3. Advanced Treatment of Raman Spectroscopy:** Polarization of Raman scattered light. Quantum mechanical interpretation Raman effect. Molecular polarizability, classical theory of Raman effect. Pure rotational Raman spectra of linear & symmetric top molecules. Raman activity of vibrations, change in size, shape or direction of polarizability ellipsoid of simple molecules. Rule of mutual exclusion, Vibrational Raman spectra and rotational fine structure. Raman investigation of phase transitions. Resonance Raman scattering. Structure determination using IR and Raman spectroscopy. Surface enhanced Raman scattering. Non-linear Raman phenomenon. Stimulated Raman scattering. Multiphoton spectroscopy.
- 4. Electronic Spectra of Molecules:** Electronic angular momentum of molecules. Spectroscopic term symbols for atoms and molecules. Photoelectron spectroscopy: Principle, light sources for UV and X-ray P.E. spectrophotometers, and its instrumentation. Position, multiplicity and fine structure of bands in P.E. spectrum. UV-photoelectron spectra of simple atoms and molecules, X-ray photoelectron spectra of gases and solids.
- 5. Mössbauer Spectroscopy:** Nuclear properties and nuclear gamma resonance, Mössbauer isotopes, Doppler effect, Mössbauer theory, isomer shift, quadrupole interactions, and magnetic splitting in Mössbauer spectrum. Effect of electronegativity in isomer shift. Application of isomer shift and quadruple splitting measurements in tin and iron complexes, detection of *cis*-, *trans*-isomer from quadruple splitting value and estimation of covalent character of complex compounds from isomer shift value.
- 6. Nuclear Magnetic Resonance Spectroscopy:** General theory of high resolution of nmr, pulse and Fourier transformation methods,

experimental techniques, double resonance methods. Relation between structure and chemical shifts, spin-spin coupling (general, vicinal and long range), Investigation of molecular fluxional properties using nmr technique.  $^{13}\text{C}$  nmr spectra, comparison with  $^1\text{H}$  nmr, hyperfine splitting, proton decoupling, interpretation of  $^{13}\text{C}$  nmr spectra. Introduction to 2D nmr, the COSY and NOESY techniques. ENDOR technique in nmr.

7. **Electron Spins Resonance Spectroscopy:** Quantization of angular momentum, relation between magnetic moment and angular momentum, characteristics of spin system,  $g$  factor, characteristics of dipolar interaction. Electronic and nuclear Zeeman interaction, spin Hamiltonian including isotropic hyperfine interaction. Isotropic hyperfine effect in esr spectra, hyperfine splitting from single set of equivalent protons multiple set of equivalent protons, hyperfine splitting from other nuclei with  $I = \frac{1}{2}$  and  $I > \frac{1}{2}$ . Zeeman anisotropy, hyperfine anisotropy. Rules of interpretation of esr spectra. esr spectrometer and scope of esr technique.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Gather information from character table.
- (ii) Explain the understanding principle of using pulse and FT-nmr techniques.
- (iii) Acquaint with spectroscopic term symbols (electronic states) of atoms and molecules.
- (iv) Get idea about Mossbauer spectroscopy, recoilless emission and absorption of  $\gamma$ -ray by the nuclei.
- (v) Realize theory of esr and ENDOR spectroscopy, cause of hyperfine and super hyperfine splitting in esr spectrum, calculation of  $g$  value and understand anisotropy in  $g$  and  $A$  values.

### Books Recommended

1. Chemical Application of Group theory, F. A. Cotton.
2. Fundamental of Molecular Spectroscopy, C. N. Banwell.
3. Introduction to Molecular Spectroscopy, G. M. Brown.
4. Electron Paramagnetic Resonance, J. A. Weil, J. R. Bolton, and J. E. Wertz.
5. Modern Spectroscopy, J. M. Hollas.
6. Introduction to Spectroscopy, D. L. Pavia and G. M. Lampman.
7. Recently Published Papers on the Above Topics in Different Journals.

**Learning Objectives**

The learning objectives of this course are to

- (i) Provide knowledge about the basic concepts of supramolecular and nano-chemistry.
- (ii) Develop capability of designing supramolecular assembly and nanoparticles and their synthesis.
- (iii) Understand the origin of non-covalent forces and their application in supramolecular chemistry.
- (iv) Learn about the properties of nanomaterials including quantum size effect and bulk behavior.
- (v) Familiarize with the modern development and applications of nano-chemistry

**Course Content**

1. **Supramolecular Chemistry:** Conceptual foundations of supramolecular chemistry, supramolecular, bioorganic, bioinorganic and biomimetic chemistry, from molecular materials to supramolecular structures, selectivity, supramolecular interactions, supramolecular design.
2. **Supramolecular Systems:** Solution host-guest chemistry: guests in solution, macrocyclic vs. acyclic hosts, cation binding, anion binding, neutral-molecule binding, self-assembly: rotaxanes, catenanes and knots, solid state supramolecular chemistry: clathrates, clathrate hydrates, crystal engineering.
3. **Organized Systems:** Surfactants, micelles, vesicles, reverse micelles, microemulsions: preorganization of surface-active compounds. Interfaces and liquid assemblies. Order in liquids, interfacial ordering, surfactants, micelles, vesicles and other ordered aggregates, surface self-assembled monolayers, supramolecular liquid crystals, ionic liquids, liquid clathrates.
4. **Nanochemistry:** About size scales, history, Feynman scorecard, Schrodinger's cat-quantum mechanics in small systems, fluctuations and "Darwinian nanoscience", quantum effects and fluctuations in nanostructures, microscopy and manipulation tools in nanochemistry.
5. **Methods for the Synthesis of Nanomaterials:** *Top-down approach:* Photolithography, electron beam lithography, micromechanical structures, thin film technologies, molecular beam epitaxy, focused ion beam milling, *Bottom-up approach:* Common aspects of all assembly methods, laser vaporization technique, chemical bath deposition method, chemical vapor deposition technique, laser ablation technique,

organic synthesis, electrodeposition, spin coating, DNA nanotechnology.

6. **Electrons in Nanostructures, Quantum Size Effect, and Bulk Behavior of Nanomaterials:** Electrons in nanostructures and quantum effect, electrons passing through tiny structures: the Landauer resistance, charging nanostructures: Coulomb blockade, resonant tunneling. The effect of the nanoparticles size on their optical and luminescent characteristics, redox properties of semiconductor nanoparticles, dependence of thermodynamic parameters of nanocrystals on their size, bulk behavior of nanomaterials. Molecular electronics.
7. **Nanostructured Materials and Their Applications:** Fullerenes; properties, aromaticity, solubility, endohedral fullerenes. Carbon Nanotube: multiwalled nanotube, single walled nanotube, electronic structure and properties. Dendrimers, fibres, gels and polymers, nanowires, molecular devices, nanostructure for electronics, photonic applications of nanoparticles, nanobiology and biomimetic chemistry, superparamagnetic nanoparticles, nanostructured thermal devices, nanofluidic devices, enhanced fluid transport in nanotubes, superhydrophobic nanostructured surfaces, nanocomposites.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Acquire fundamental knowledge on supramolecular assembly and nano-chemistry.
- (ii) Realize the non-covalent forces and their applications in supramolecular chemistry.
- (iii) Gain knowledge on design, synthesis and applications of supramolecular and nano-chemistry.
- (iv) Understand the self-assembly in molecular levels including biological self-assembly.
- (v) Familiarize with nanostructured materials such as fullerenes, carbon nanotube, etc. and their applications.

### Books Recommended

1. Supramolecular Chemistry, F. Vogtle.
2. Supramolecular Chemistry, J. W. Steed and J. L. Atwood.
3. Core Concepts in Supramolecular Chemistry and Nanochemistry, J. W. Steed, D. R. Turner and K. J. Wallace.
4. Introduction to Nanoscience, S. M. Lindsay.
5. Nanostructures and Nanomaterials: Synthesis, Properties and Applications, G. Cao.
6. Fullerenes: Chemistry and Reactions, A. Hirsch, M. Brettreich and F. Wudl.

### Learning Objectives

The learning objectives of this course are to

- (i) Provide with a basic understanding of the various materials used in engineering applications.
- (ii) Acquire knowledge on basics of material science, structure and property relationships for polymers, metals, and ceramics, advanced materials.
- (iii) Describe phase equilibria of materials and the microstructure involved during phase changes.
- (iv) Design and synthesis of new materials including composites..

### Course Content

1. **Materials:** Materials science and engineering, classification of materials, materials of the future, smart and intelligent materials, nanotechnology, modern materials' needs.
2. **Mechanical Properties of Materials:** Concept of stress and strain, elastic deformation, stress-strain behavior, anelasticity, elastic properties of materials, tensile properties, plastic deformation, tensile properties, true stress and strain, elastic recovery after plastic deformation, compressive, shear, and torsional deformations, hardness. Variability of material properties, design/safety factors, dislocation, characteristics of dislocations, slip, slip systems, generalized creep behavior, stress and temperature effect, viscoelastic deformation.
3. **Thermal and Electrical Properties of Materials:** Heat capacity, thermal expansion, materials of importance-Invar and other low expansion alloys, thermal conductivity and thermal stresses, thermal protection system on the space shuttle orbiter, electrical conduction, semiconductivity, temperature dependence of carrier concentration, factors that affect carrier mobility, Hall effect, semiconductor devices, electrical conduction in ionic ceramics and in polymers, dielectric behavior, capacitance, field vectors and polarization, types of polarization, frequency dependence of the dielectric constant, dielectric strength, dielectric materials, ferroelectricity, piezoelectricity, conducting polymers, polymer electrolytes; interaction between polymer and salts, polymer in salt and salt in polymer electrolytes.
4. **Magnetic Materials:** Basic concepts, diamagnetism and paramagnetism, ferromagnetism, antiferromagnetism and ferrimagnetism. Influence of temperature on magnetic behavior, domains and hysteresis, magnetic anisotropy, soft and hard magnetic materials, magnetic storage, superconductivity, superconducting quantum interference device.

5. **Optical Properties of Materials:** Light interactions with solids, atomic and electronic interactions, optical properties of metals, optical properties of nonmetals, refraction, reflection, absorption, transmission, color, opacity, and translucency in insulators, applications of optical phenomena, luminescence, materials of importance- light emitting diodes (LED), photoconductivity, lasers, optical fibers in communications; components, step index, graded index optical fiber design.
6. **Phase Diagrams and Microstructure in Materials:** Definitions and basic concepts, binary phase diagrams, binary isomorphous systems, interpretation of phase diagrams, development of microstructure in isomorphous alloys, mechanical properties of isomorphous alloys, binary eutectic Systems, materials of importance- lead-free solders. Ceramic and ternary phase diagrams, Gibbs phase rule, development of microstructure in eutectic alloys, equilibrium diagrams having intermediate phases or compounds, eutectic and peritectic reactions, congruent phase transformation, iron-iron carbide phase diagram, development of microstructure in iron-carbon alloys; Superalloys.
7. **Composite Materials:** Particle-reinforced composites: large-particle composites, dispersion-strengthened composites, fiber-reinforced composites: influence of fiber length, influence of fiber orientation and concentration, the fiber phase, the matrix phase, polymer-matrix composites, metal-matrix composites, ceramic-matrix composites, carbon-carbon composites, processing of fiber-reinforced composites, hybrid composites, structural composites: laminar composites, sandwich panels, materials of importance- nanocomposites in tennis balls, biomaterials and advanced ceramics.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Describe processing, structure, property and performance of material.
- (ii) Explain the basic properties and characteristics of metals, polymers and ceramics, etc.
- (iii) Realize basic concepts of phase equilibria of materials and understand the changes in microstructures involved during phase changes and transformation.
- (iv) demonstrate the basic aspects of advanced materials and their applications, such as electronic materials, optical materials, and magnetic materials
- (v) Design new materials including composite materials and select the proper materials for application in multidisciplinary areas.

## Books Recommended

1. Materials Science and Engineering: An Introduction, W. D. Callister.
2. The Science and Engineering of Materials, D. R. Askel and P. Phulé.
3. Foundations of Materials Science and Engineering, W. F. Smith.
4. Solid Polymer Electrolytes, F. M. Gray.
5. Physical Chemistry, P. W. Atkins and J. D. Paula.
6. Ionic Liquids in Polymer Systems, R. D. Rogers and C. S. Brazel.

## PC 510 Advanced Concepts of Liquids

(3 Credits)

### Learning Objectives

The learning objectives of this course are to

- (i) Understand recent concepts and acceptable models of structure of liquid state.
- (ii) Understanding of possible intermolecular forces among the molecules of liquids.
- (iii) Illustrate the important physical properties of liquids, such as: viscosity, surface thermodynamic properties, dielectric constant, etc. and their measurement techniques.
- (iv) Discuss the physicochemical properties of liquid crystals and ionic liquids.

### Course Content

1. **Theories and Concepts of Liquid State:** Cluster theory, optimized cluster theory: the Lennard-Jones fluid, X-rays and the solid like state theory of liquids, distribution of molecules in liquids, Monte Carlo method of molecular distribution in liquid: radial distribution functions. Models of liquid: microscopic model, Cybotactic group model, kinetic molecular model, liquid as a modified solid, Bernal's random close-packed model, hard sphere model, lattice model and defect solid state model.
2. **Intermolecular Forces in Liquids:** Nature of intermolecular forces in liquid. Different types of forces- their mathematical expression and resulting effect: dipole-dipole forces (orientation effect), dipole-induced dipole interaction (induction effect), instantaneous dipole-induced dipole interaction (dispersion effect), repulsive interaction, total potential energy of a pair of liquid molecules and its comparison with repulsive interaction, hydrogen bonding, different types of hydrogen bonding in water, structure of water (cluster to bulk).
3. **Viscous Flow of Liquids:** Maxwell's theory of gas viscosity, difference between the mechanism of gas and liquid viscosity: Lord Rayleigh and Chapman and Enskog contributions. Viscous flow of

liquids: Navier-Stokes equation, Newtonian and non-Newtonian liquids. Thermodynamic activation parameters of liquids, viscosity of mixtures. Types of fluids on the basis of viscous flow of liquids.

4. **Nature and Thermodynamics of Liquid Surfaces:** Surface thermodynamic quantities and the temperature dependence of surface free energy, the total surface energy, change of vapor pressure for a curved surface (Kelvin equation), effect of curvature pressure and other variables on surface tension, contact angle and adhesion, surface concentration (Gibb's equation), surface film, surface equation of state.
5. **Liquid Crystals:** Liquid crystallinity: classification and properties, structural features, mesomorphic state, isotropic liquid, mesophase, different types of mesophase, smectic mesophase and their properties, amphiphilic and non-amphiphilic mesogens. Conversion of different types of mesogens. Lyotropic, thermotropic, helical nematic-choleic and columnar phase liquid crystals. Theory of liquid crystals: molecular order, order tensor, chemical structure and thermal stability, idealized structure of a calamitic liquid crystal. Applications of liquid crystals. Polymeric liquid crystals and ferroelectric liquid crystals. Theories of phase transition: molecular field theory (Onsager's model, Maier-Saupe model), mean field theory, the Landau theory, Landau-de Gennes free energy, McMillan theory and its extension.
6. **Ionic Liquids:** Definition, attraction of ionic liquids; cations and anions in ionic liquid; types of ionic liquids; structure of ionic liquids, ionicity of ionic liquids, synthesis of ionic liquids, properties of ionic liquids, ionic liquids as designer solvents; green credentials of ionic liquids, use of ionic liquids in electrochemistry and catalysis.
7. **Experimental Techniques for Investigations of the Structures of Liquids:** Viscosity: Falling ball viscometer and Ladenburg correction, Cannon-Finske viscometer, Ostwald viscometer. Surface tension: direct measurement using microbalance (Wilhelmy plate, du Noüy ring method), measurement of capillary pressure (maximum bubble pressure and growing drop method), analysis of capillary gravity force (capillary rise and drop volume method), gravity-distorted drops (Pendent drop and sessile drop methods), reinforced distortion of drop (spinning drop and micropipette methods). Dipole moment: from relative permittivity and refractive index, Heterodyne-beat method.

## Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Illustrate different modern theories and models of liquid.
- (ii) Demonstrate on different possible intermolecular forces among the molecules of liquids.

- (iii) Explain important properties of liquids, such as; viscosity, surface thermodynamic properties, dielectric constant, etc. and their theoretical basis of measurements.
- (iv) Synthesize and use liquid crystals and ionic liquids for different purposes based on their physicochemical properties.

### Books Recommended

1. Molecular Theory of Gases and Liquids, J. O. Hirschfelder, C. F. Curtiss and R. B. Bird.
2. Physical Chemistry of Surface, A. W. Adamson and A. P. Gast.
3. Physical Properties of Molecular Crystals Liquids and Glasses, A. Bondi.
4. The Structure and Properties of Solution, Discussion of Faraday Society, Chemical Society, London, **43**, 1967.
5. An Introduction to Ionic Liquids, M. Freemantle.
6. Supramolecular Chemistry, F. Vogtle.

### PC 511 Advanced Polymer Chemistry

(3 Credits)

#### Learning Objectives

The learning objectives of this course are to

- (i) Provide basic understandings on different kinds of polymerization techniques and mechanisms
- (ii) Give idea about commercially important and functional polymers in industry and research.
- (iii) Aware of advanced techniques of characterization, commercial utilizations of polymers and their environmental impact.
- (iv) Impart knowledge on polymer modification and processing.

#### Course Content

1. **Kinetics of Polymerization - Free Radical Polymerization:** Free radical initiators, kinetics and mechanism of polymerization, kinetic chain length, chain transfer agents, atom transfer radical polymerization (ATRP), reversible addition fragmentation termination (RAFT). **Step reaction polymerization:** Kinetics of step reaction polymerization, Carother's equation, stoichiometric imbalance, reactivity and molecular size. Dendritic polymers, ring-opening polymerization. **Ionic and coordination polymerization:** Cationic and anionic polymerization, mechanism of cationic and anionic polymerization, living polymers. Mechanism of coordination polymerization– Ziegler-Natta catalysts.
2. **Polymer Reaction Engineering:** Introduction, polymerization processes, homogeneous systems-bulk polymerization, solution polymerization, heterogeneous polymerization-suspension

polymerization, emulsion polymerization, precipitation polymerization, interfacial and solution polycondensations, polymerization reactors, batch reactors, tubular (plug flow reactor), continuous stirred tank reactor.

3. **Functional Polymers:** Conducting polymers, polymer liquid crystals, polymers in lithography, polymer composites and nanocomposites, polymer gels; hydrogels, stimuli sensitive hydrogels, self-oscillating polymer gel, controlled release drug delivery polymer hydrogels, polymer in optoelectronics, polymer blends and alloys, click polymerization-combination of living radical polymerization and click chemistry, self-healing polymers, self-assembling polymers, inorganic polymers.
4. **Polymer Modification:** Copolymerization: styrene-butadiene copolymers, styrene-butadiene rubber (SBR) (random copolymer), styrene-butadiene block polymers, ethylene copolymers, acrylonitrile-butadiene-styrene copolymers (ABS), condensation polymers: acetal copolymer, epoxies, urea-formaldehyde (UF) resins. Post polymerization reactions: reactions of polysaccharides, cellulose derivations, starch and dextrans, cross-linking, unsaturated polyesters, block and graft copolymer formation, surface modification.
5. **Polymer Processing:** *Plastic technology:* Molding – compression molding, transfer molding, injection molding, RIM, blow molding, rotational molding, thermoset molding. Extrusion – coextrusion, film extrusion, pultrusion. *Fiber technology:* Textile and fabric properties – Definition of textile terms, properties of textile fibers – electric, mechanical and fabric properties. Spinning – melt spinning, dry spinning, and wet spinning. *Elastomer technology:* elastomers properties, Vulcanization – chemistry of vulcanization, physical aspects. *Polymer additives and reinforcements:* Plasticizers, fillers and reinforcements, alloys and blends, antioxidants and thermal and UV stabilizers, flame retardants, colorants, antistatic agents.
6. **Characterization Techniques of Polymers:** UV, IR and RAMAN,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and mass spectroscopy: characteristic absorption of organic monomers and polymers, UV spectral data for polymer characterization, IR spectra of organic monomers and polymers, structural characterization of polymers by IR (and Raman) spectroscopy, polymer pyrolysis, GC-MS, FABMS technique, MALDI-TOF. Thermogravimetric analysis (TGA). Differential thermal analysis (DTA), differential scanning calorimetry, dynamic-mechanical analysis (DMA), thermo-mechanical analysis (TMA).
7. **Polymer in Wastes and Their Environmental Impact:** Polymer industry and environment. Natural resources scenario, waste items,

classified waste materials, power scenario, municipal solid wastes, waste management, recovery and recycling of organic wastes, composting, sortation, micro-sortation, polymer reprocessing. Polymer incineration. Integrated waste management for sustainable development.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Gather detailed knowledge on kinetics and mechanism involved in polymerization reactions.
- (ii) Acquire insight into different techniques and reactors used in polymer synthesis, and the industrial processes involved.
- (iii) Characterize polymers and discuss their structural, thermal, and mechanical properties.
- (iv) Apply knowledge on sortation, and disposal of polymers.

### Books Recommended

1. Textbook of Polymer Science, F. W. Billmeyer.
2. Polymer Chemistry, M. P. Stevens.
3. Polymer Science and Technology, R. O. Ebewele.
4. Polymer Science and Technology, P. Ghosh.
5. Polymer Chemistry, P. C. Hiemenz and T. P. Lodge.
6. Polymer Science, V. R. Gowariker, N. V. Viswanathan and J. Sreedhar.

## PC 512 Computational Chemistry

3 (Credits)

### Learning Objectives

The learning objectives of this course are to

- (i) Discuss the principles of quantum mechanics, involving atoms, molecules and their chemical reactions.
- (ii) Impart knowledge on eigenvectors and eigen values, the Schrodinger equation, orbitals, and variational and perturbational methods.
- (iii) Acquire knowledge on different methods for the calculation of molecular properties and comparison of these methods. .

### Course Content

1. **Time Independent Perturbation Theory and Variational Methods.**
2. **Molecular Electronic Structure:** Born-Oppenheimer approximation, potential energy surface, molecular orbital picture / LCAO, Slater-Condon Rules, SCF wave function, electron correction: (i) configuration-interaction,
3. **Computational Methods:** (1) molecular mechanics, (2) *ab initio* methods: (i) SCF theory, (ii) post Hatree-Fock theory and (3) density functional theory: Principle and applications.

4. **Methods for Simulating Large System:** (A) Non-bonded cutoff, (B) Boundaries, and (C) long-range interactions: The Ewald summation and the reaction field method.
5. **Energy Minimization Techniques:** Steepest descent, Conjugate gradient and Newton-Raphson, and comparison of the methods.
6. **Monte Carlo (MC):** (i) MC integration and Markov chain and (ii) the metropolis method.
7. **Molecular Dynamics:** (i) Classical mechanics: Equation of motion, (ii) Finite Difference method and (iii) constrained dynamics.

### **Learning Outcomes**

Upon completion of this course, the students will be able to

- (i) Gain knowledge on the laws of quantum mechanics involving atoms, molecules and their chemical reaction.
- (ii) Explain potential energy surfaces and hypersurfaces, geometry optimization, stationary points and saddle points.
- (iii) Capable of applying appropriate methods for calculation of problems involved in a chemical reaction

### **Books Recommended**

1. AB Initio Molecular Orbital Theory, W. J. Hehre, L. Radele, P. R. Schleyer and J. A. Pople.
2. Modern Techniques in Computational Chemistry, E. Clementi.

## Detailed Syllabus for M. S. (Thesis Group) in Organic Chemistry

### ORG 521 Advanced Reaction Mechanism

(3 Credits)

#### Learning Objectives

The learning objectives of this course are to

- (i) Review the concepts of hard and soft acids and bases extending to ambient electrophiles and ambient nucleophiles.
- (ii) Impart detailed knowledge on Molecular Orbital (HMO) and Frontier Orbital (HOMO and LUMO) concepts and their applications to evaluate and interpret different reactions.
- (iii) Give knowledge on quantitative correlation of acidity and basicity of organic molecules and their effect on reaction rates, equilibria, substituents using different proposed equations such as Hammett equation, Yukawa-Tsuno equation etc.
- (iv) Impart knowledge on kinetics and reaction mechanism of substitution reaction, addition reaction, catalytic reaction and free radical reactions.
- (v) Give knowledge on the reaction mechanism of the medium and large ring compounds and non-benzoid aromatic compounds.

#### Course Content

1. **Acids and Bases, Nucleophiles and Electrophiles:** Definitions, ionisations, effect of solvents, effect of structure, classification on the basis of the structures of organic molecules; hard and soft acids and bases (HSAB) principle; hard and soft nucleophiles and electrophiles; ambident electrophiles and ambident nucleophiles.
2. **Molecular Orbitals and Frontier Orbitals:** Hückel molecular orbital (HMO) method. Evaluation of aromaticity and the  $4n+2$  rule in terms of HMO method. Prediction of thermal and/or photochemical reactions on the basis of aromatic and Möbius transition state concept. Calculation of resonance energy by using  $\alpha$  (coulomb integral) and  $\beta$  (resonance integral). Frontier orbital theory; HOMO and LUMO; perturbation theory of reactivity; the  $\alpha$ -effect; interpretation of ionic, pericyclic and radical reactions in terms of frontier orbital theory.
3. **Quantitative Correlation of Acidity and Basicity:** Quantitative correlation of reaction rates and equilibria, general approach, correlation with *meta*-, and *para*-substituted benzene derivatives, correlation with relatively rigid non-aromatic compounds, deviation from Hammett equation. Quantitative correlation with acidity and basicity. Derivation of Hammett equation; Hammett's  $h_o$  function; Grunwald-Winstein acidity scale, polar effects in aliphatic compounds-Taft treatment. Linear Free Energy Relationship- Hammett plots, Hammett equation, substitution constants ( $\sigma_x$ ), reaction constant ( $\rho$ ),

significance of  $\sigma_x$ , and  $\rho$ . Calculation of  $k$  and  $K$  values, deviation from Hammett-straight-line plots. Yukawa-Tsuno equation, Taft equation, Grunwald-Winstein equation. Thermodynamic implications of all these equations.

4. **Kinetics and Energetics in Reaction Mechanism:** Consecutive reactions-the steady-state approximation; parallel reactions, reversible reactions, derivation of the rate expressions, variation in kinetics in acid and base-catalyzed reactions; ambiguities in interpreting kinetic data; microscopic reversibility, correlation of reaction rates and equilibria.
5. **Substitution Reactions:** Comprehensive treatment of solvolytic reactions; substitution reactions of ambident nucleophiles; attempted correlation of substitution rates- the Swain-Grunwald equation; the Hammett equation and correlation with *meta*- and *para*-substituted benzene derivatives.
6. **Addition Reactions:** Multi-centre addition reactions - Diel's-Alder and *Retro* Diel's-Alder reactions, various types of dienes, and dienophiles, 1,3-dipolar additions, chelotropic reactions, and their stereochemistry, nucleophilic addition to C=O group (the Cram's rule, stereochemical treatment) and related unsaturated system
7. **Catalysis:** Acid-base catalysis, definitions and examples, mechanisms of acid and base-catalyzed reactions, rate of acid and base-catalyzed reactions. Classification of catalysts - electrophilic and nucleophilic catalysis, "physical" catalysis, acid-base catalysis, intramolecular catalysis, enzymic catalysis, catalysis of non-ionic reaction mechanisms.
8. **Molecular Rearrangement:** Carbocation rearrangements in bridged-bicyclic system - the norbornyl systems treating both classical and non-classical carbocations showing how anchimeric assistance plays its role. Rearrangements in small-ring compounds.
9. **Chemistry of Medium and Large-ring Compounds:** *Transannular* reactions.
10. **Chemistry of Non-Benzenoid Aromatic Compounds:** Azulenes and annulenes.
11. **Mechanism of Free Radical Reactions:**  
*Part I: Long-lived and short-lived free radicals* - configuration of free radicals, generation and detection of free radicals, types of free radical reactions and some of their common characteristics.  
*Part II: Homolysis and free radical displacements* - Iodine-exchange reactions, autoxidations, decomposition of various peroxides, azo and diazo compounds.  
*Part III - Additions and rearrangements of free radicals.*

## Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Demonstrate the knowledge on hard and soft acids and bases extending to electrophiles and nucleophiles and their quantitative relationship.
- (ii) Understand the molecular orbital theory and orbital symmetry of organic molecules and appreciate both structural and chemical transformation of organic molecules.
- (iii) Understand the involved kinetics and energetic of reaction mechanism.
- (iv) Explain reaction mechanism of different types of reaction such as substitution, addition, catalytic, and free radical reactions.

## Books Recommended

1. Mechanism in Organic Chemistry, R. W. Alder, R. Baker and J. M. Brown.
2. Frontier Orbitals and Organic Chemical Reactions, I. Fleming.
3. Mechanism and Structure in Organic Chemistry, E. S. Gould.
4. Organic Reaction Mechanisms: An Introduction, R. Breslow and W. A. Benjamin.
5. Organic Chemistry, S. H. Pine, J. B. Hendrickson, D. J. Cram, and G. S. Hammond.
6. Physical Organic Chemistry, N. S. Isaacs.
7. Physical Organic Chemistry, J. Hine.

## ORG 522 Advanced Stereochemistry

(3 Credits)

### Learning Objectives

The learning objectives of this course are to

- (i) Provide the fundamental concepts on symmetry, symmetry operations, symmetry and molecular properties, molecular dissymmetry etc.
- (ii) Impart knowledge on chiroptical properties, factors leading chirality. Application of different techniques and rule for the determination of structure, conformation and configuration.
- (iii) Have knowledge on stereochemistry of trivalent carbon, optical activity due to atoms other than carbon, prostereoisomerism, prochirality and pseudochirality.
- (iv) Impart knowledge on chirality in molecules devoid of chiral centres.
- (v) Convey knowledge on asymmetric synthesis.

### Course Content

1. **Optical Rotation and Rotatory Power (Chiroptical Properties):** Factors leading to chirality. Elements of symmetry, Molecular symmetry and group theory. Molecular dissymmetry. Atomic asymmetry and conformational asymmetry. *Circular birefringence* and

*circular dichroism (CD). Optical rotatory dispersion (ORD). Cotton effect. Description of ORD curve. Haloketone rule and Octant rule. Application of these in determining the structure, conformation and configuration of different compounds. Optical Rotation and Rotatory Power (Chiroptical Properties).*

2. **Symmetry:** Introduction, symmetry elements, symmetry operations, symmetry point-groups, desymmetrisation, average symmetry, symmetry and molecular properties, symmetry numbers.
3. **Conformational Analysis:** Conformation and reactivity in alicyclic, cyclic, fused and bridged ring systems (heterocyclics, decalins, anthracenes, phenanthrenes, pentalanes and propellanes, catenanes, rotaxane, knot, mobius strip, cubane, tetrahedrane, dodecahedrane, adamantane and buckminsterfullerene). Conformational effects in small, medium and large ring systems. *Curtin Hammett principle*, its application in determining the course of reaction.
4. **Stereochemistry of Tricovalent Carbons:** Carbonium ions and carbanions.
5. **Optical Activity due to Atoms Other Than Carbon:** Nitrogen, phosphorus, arsenic, sulphur, selenium and other chiral compounds.
6. **Prostereoisomerism, Prochirality and Pseudochirality:** Introduction, terminology, significance, history. Chiral, prochiral, and pseudochiral molecules, pro-R, pro-S, homotopic and heterotopic ligands and faces; enantiotopic ligands (HCN addition), diastereotopic ligands and faces, heterotopic ligands and faces in enzyme-catalyzed reactions, heterotopicity and nuclear magnetic resonance.
7. **Chirality in Molecules Devoid of Chiral Centres:** Atropisomerism, nomenclature, synthesis and stereochemistry of Biphenyls, Allenes, Cyclic allenes and Spiranes. Molecules with planar chirality.
8. **Asymmetric Synthesis:** Introduction, diastereoselective synthesis, *Cram's rule*, enantioselective synthesis, double stereodifferentiation.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Demonstrate on chiroptical properties, factors leading to chirality, and apply different techniques and rules for the determination of structure, conformation and configuration.
- (ii) Understand stereochemistry of trivalent carbon, optical activity due to atoms other than carbon, prostereoisomerism, prochirality and pseudochirality.
- (iii) Find out chirality in molecules devoid of chiral centres and carry out asymmetric synthesis.

## Books Recommended

1. Stereochemistry of Carbon Compounds, E. L. Eliel.
2. Stereochemistry of Organic compounds, L. E. Eliel and S. H. Wilen.
3. Stereochemistry: Conformation and Mechanism, P. S. Kalsi.
4. Stereoselective Synthesis in Organic Chemistry, Atta-ur-Rahman and Z. Shah.

## ORG 523 Spectroscopic Methods in Organic Chemistry (3 Credits)

### Learning Objectives

The learning objectives of this course are to

- (i) Review their knowledge about different types of spectroscopic technique i.e., UV, IR, NMR and MS.
- (ii) Impart knowledge on advanced techniques about one dimension and two dimension NMR studies.
- (iii) Understand advanced techniques about mass spectrometry and its application.
- (iv) Develop skill for analyses of UV-Visible, IR and NMR and Mass spectral data to elucidate the structure of organic compounds.

### Course Content

1. **UV, IR, Raman and ESR Spectra:** Review of theory and experimental techniques, application in the identification of organic molecules and free radicals.
2. **NMR Spectrum:** Theory, experimental method, spin-spin coupling-AB system, ABX and ABX<sub>2</sub> systems. Internal rotation and the equivalence and non-equivalence of nuclei; variable temperature spectra, factors affecting coupling constants. Dynamic nuclear magnetic resonance. Chemically induced dynamic nuclear polarization, Relaxation effect, Spin-Lattice relaxation. Measurement of T<sub>1</sub>. Mechanism of spin-lattice relaxation, Application of Dipolar Relaxation Times, Spin-Spin Relaxation, The multiple Irradiation Techniques, Spectral simplification. Elimination of Quadrupolar effects. Multiple pulse sequence, Measurement of T<sub>2</sub>, Spectral editing, Signal and resolution enhancement, Connectivity. Two dimensional NMR, COSY, NOESY, SECSY, EXTASY, INADEQUATE and RELAY experiments. COLOC experiments, HSQC, DEPT, HMBC, TOCSY & HETCOR experiments. Introduction to Tactics strategies of structure elucidation by one and two-dimensional NMR skeletal structure (atom connectivities) by NMR experiments. Relative configuration and conformation by NMR. <sup>13</sup>C-NMR and theoretical calculation of <sup>13</sup>C value. Applications of NMR in the structure elucidation of organic compounds.

3. **Mass Spectroscopy:** Theory, spectrometer and application to structure determination of organic molecules. Kinds of mass spectrum: Electron Impact (EI) and Chemical Ionization (CI), Fast Atom Bombardment (FAB), Secondary Ion Mass Spectroscopy (SIMS), Electron Spray (ES) and Thermo Spray (TS) spectra, Matrix Assisted Laser Ionization / Desorption (MALDI), Field Desorption (FD) and Plasma Desorption (PD). Tandem Mass Spectroscopy (MS-MS / MS-MS-MS). Analyzer: Magnetic Sector, Quadrupole, Ion Trap, Time-Of-Flight (TOF), Fourier Transform-ion Cyclotron Resonance (FTICR or FTMS). 3D-Mass spectroscopy. Circular dichroism (CD) and its application in configurational studies.
4. **Following Progress of Reactions by Spectroscopy:** Diagnostic appearance and disappearance of functional groups in organic compounds and also in characterizing the products.
5. **Structure Elucidation by Spectroscopy:** Joint application of UV, IR, NMR, and mass spectroscopy in the structure elucidation of organic compounds- illustration with the spectra of typical compounds.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Identify compounds by analysis and interpretation spectral data.
- (ii) Analyze and interpret 1D and 2D NMR spectra.
- (iii) Learn how to use modern mass spectrometry techniques (CI, ESI, FAB, TOF, GC-MS, LC-MS/MS) to find out the molecular mass and structure.
- (iv) Acquire the ability to determine the structure of typical organic compounds using spectroscopic techniques.

### Books Recommended

1. Spectroscopic Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill.
2. Spectroscopic Methods in Organic Chemistry, D. H. Williams and I. Fleming.
3. Spectroscopic Analysis, D. L. Pavia, G. M. Lampman and G. S. Kriz.
4. Basic One- and Two-Dimensional NMR Spectroscopy, H. Friebolin.
5. Introduction to Mass Spectrometry, H. C. Hill.

## ORG 524 Separation and Chromatographic Techniques (3 Credits)

### Learning Objectives

The learning objectives of this course are to

- (i) Impart knowledge on chromatography and its basic principle for separation, identification and quantification of organic compounds.
- (ii) Give knowledge on TLC using different stationary phases.
- (iii) Impart knowledge on some advanced systems of chromatographic techniques such as DCCC, MLCCC, SPE etc.
- (iv) Impart knowledge on various gas chromatographic techniques, their working principle, instrumentation and applications with different detectors.
- (v) Demonstrate advanced knowledge on HPLC with different detectors and their application for separation, identification and quantification of organic compounds.
- (vi) Provide the principle and applications of LC-MS.

### Course Content

1. **Chromatographic Techniques:** Chromatography and its basic principles: adsorption, partition, size exclusion, ion exchange and affinity chromatography. Column chromatography, gravitational chromatography, flashes chromatography, and vacuum liquid chromatography (VLC), Stationary phases for column chromatography: normal and reversed phase, bonded phase etc. Stationary phase for size exclusion chromatography. Column, void and dead volume in column chromatography. Column efficiency and theoretical plate, resolution, elution pattern, frontal analysis, retention time and phase distribution constant, retention factor and selectivity factors in separation.
2. **Ion-Pair Chromatography:** Theory of ion-pair separation in liquid chromatography (LC), ion pairing reagents, ion pairing in ion-exchange and ion-suppression mode. Effect of buffer and pH in ion-pair chromatography.
3. **Review of Thin-layer and Paper Chromatography:** Principles and application, Preparative Thin Layer Chromatography (PTLC), High Performance Thin Layer Chromatography (HPTLC) and its components. Identification and quantification of organic compounds by HPTLC.
4. **Some Advanced Systems of Chromatography:** Centrifugal chromatography - Chromatotron; Droplet Counter Current Chromatography (DCCC), Multilayer Counter Current Chromatography (MLCCC), Solid Phase Extraction (SPE) Chromatography (normal and reversed phase). Application of SPE in purification and clean-up of organic compounds.

5. **Gas Chromatography (GC):** Gas chromatograph: gas chromatograph and its components. Gas solid Chromatography (GSC), Gas Liquid Chromatography (GLC). Carrier gas, Injectors - manual and auto-injector; Split and Split/ splitless glass liner of GC, types of detector: Universal Detector & Specific detector. Thermal Conductivity Detector (TCD), Flame Ionization Detector (FID), Electron Captured Detector (ECD). Nitrogen Phosphorus Detector (NPD), Mass Detector (MSD), GC-IR & MS, GC with biological & Mass detectors. Cross sectional diagram, function, detection limit, linearity, sensitivity and specificity of each detector. Different types of column of GC: non polar, medium polar and polar phases. Isothermal and temperature programme of elution. Theoretical plates, length and diameter of column on resolution, Influence of temperature of resolution. Identification and quantification, method development and validation for analysis by GC.
6. **Gas Chromatography and Mass Spectrometry (GC-MS):** Selective Ion Mode (SIM) and SCAN; identification-fragment pattern and library search. Quantification by SIM and SCAN method. Common trouble shooting in operating GC and GC-MS. Use of GC for organic compound.
7. **High Performance Liquid Chromatography:** An overview of LC and its components: Solvent reservoir, higher and low pressure pumps, gradient programmers, column at ambient temperature & oven, detector and data processing unit. Different types of LC: Ultra performance (UPLC) liquid chromatography, Capillary liquid chromatography (micro-HPLC), Capillary electro chromatography (CEC) and Medium pressure liquid chromatography (MPLC), Different types of detectors of LC: UV-VIS: Fixed wave length, variable wave length, Photodiode array, Fluorescence, Electrochemical, Dielectric constant, Refractive index, Light scattering mass and MS detectors: Function of each detector, sensitivity, linear dynamic range and response index, class of compound to be separated by each detector. Advantages and limitations of each detector. Size of column, particle, pressure and temperature in UPLC. Chiral and ion exchange LC separations. Identification and quantification, method development and method validation for analysis by LC. Use of LC-NMR in drug discovery.
8. **Liquid Chromatography and Mass Spectrometry (LC-MS) Ionization Techniques:** Electro Spray Ionization (ESI), Atmospheric Pressure Chemical Ionization (APCI), Atmospheric Pressure Photo Ionization (APCI), Dual sources (ESI/APCI) or (APCI/APPI) system of ionization. Ionization Source Principles: Production of charged droplets, Evaporation, Droplet size reduction, and fission (Coulomb explosion), gas phase ion formation, clustering and declustering, curtain gas, corona charged needle etc. Mass Analyzer: Triple

Quadrupoles (QQQ), Ion Trap (IT) and Hybrids (e.g. LIT). Identification and quantification of compounds by LC-MS. Effect of acids or bases in ionization process. LC-MS-MS systems: Ion trap (traditional special traps), Triple quadruple (QQQ), and Q-trap systems. Specificity and sensitivity of LC-MS and LC-MS-MS; Comparison of LC with LC-MS; LC-MS with LC-MS-MS. Common trouble shooting in operating LC, LC-MS and LC-MS-MS. Identification and quantification, method development & validation for analysis by LC-MS.

9. **Supercritical Fluid Chromatography:** Properties of supercritical fluids, effects of pressure, stationary and mobile phase, comparison of SPC with other chromatographic methods.

### Learning Outcomes

Upon completion of this course, the student will be able to

- (i) Understand the basic principles of various chromatographic techniques and demonstrate different related terms.
- (ii) Acquainted with the principles and application of paper, thin layer and ion-pair chromatographic techniques.
- (iii) Apply chromatographic techniques such as HPLC, GC and GC-MS for the separation, identification, and quantification of organic molecules using different detectors.
- (iv) Demonstrate and apply knowledge on analyzing various types of samples using LC-MS.
- (v) Review and compare some advanced chromatographic techniques for their application in different organic samples.

### Books Recommended

1. Practical Liquid Chromatography, S. G. Perry, R. Amos and P. I. Brewer.
2. Analytical Chemistry Principles, J. H. Kennedy.
3. Chemical Analysis, H. A. Laitinen.
4. Fundamentals of Analytical Chemistry, D. Skoog, D. M. West and F. G. Holler.
5. High Performance Liquid Chromatography, S. Lindsay.
6. Instrumental Methods of Chemical Analysis, G. W. Ewing.
7. Modern Methods of Chemical Analysis, R. L. Pecsok and L. D. Shields.
8. Analytical Chemistry, G. D. Christian.
9. Practical HPLC, V. R. Meyer.
10. HPLC, A practical guide, T. Hanai.
11. Analytical Chemistry Handbook, J. A. Dean.

### Learning Objectives

The learning objectives of this course are to

- (i) Provide basic concepts on the strategy for carrying out an organic synthesis process.
- (ii) Impart knowledge for developing ability to plan and carry out synthetic experiments independently.
- (iii) Grow critical awareness of advances at the forefront of new methodologies in the synthesis of biologically important organic molecules.

### Course Content

1. **The Importance of Synthetic Organic Chemistry:** Planning of organic synthesis and choosing of synthesis route. *Strategy in Synthesis:* The disconnection approach to synthesis, concept of a synthon, synthetic equivalent and target molecule: Synthesis of monofunctional and difunctional compounds: (i) One-group disconnection: disconnection of simple alcohols -compounds derived from alcohols, disconnection of simple olefins, ketones. (ii) Two group disconnections: 1,3- dioxigenated skeletons
2. **Reaction Intermediates in Organic Synthesis with Particular Reference to:** Carbenes, ketenes and nitrene (electronic structure and energy, generation reaction type chemical activation, structure and reactivity). Enamines and heterocyclic enamines.
3. **Organometallic Reagents in Organic Synthesis:** The principles, reactions of organometallic compounds, Grignard reagents, organo copper reagents, formation of carbon -hetero atom bonds, unpolung, ylides, stereoselective enolate reactions, Michael addition and Robinson annulations; Heck reactions and Suzuki reaction.
4. **Oxidation and Reduction Methods in Synthesis:** Dissolving metal reduction, reduction with hydrazine and its derivatives, (system containing nitrogen and sulphur), reduction with lithium aluminium hydride and sodium borohydride, oxidation with chromium and manganese compounds, peracids and peroxides, mercuric acetates and selenium dioxide, (hydrocarbons and system containing oxygen, nitrogen and sulphur), oxidation with lead tetraacetate and periodic acid.
5. **Interconversion of Functional Groups:** (a) Interconversion of functional groups, transformation of alcohols, phenols, halogenocompounds, nitro-compounds, acids and acid derivatives to other compounds, (b) protective groups: the strategy of using protective

groups, application of protective groups in the protection of alcohols, diols, carboxylic acid, amino groups, carbonyls groups in organic synthesis, addition and removal of carbon atom in organic synthesis.

6. **Stereoselective Synthesis:** Regioselective, diastereoselective and enantioselective synthesis, synthesis chiral compounds, optical purity and enantiomeric excess, chiral catalyst, solvent and reagents.
7. **Design of Drug Synthesis:** Synthesis of stereospecific drugs. Making single enantiomers, structure activity relationship, use of retrosynthesis in designing synthesis of biologically important organic compounds. Synthesis of some typical medicinal compounds - ascorbic acid,  $\beta$ -carotene, penicillin, cephalosporin C, prostaglandins ( $F_{2\alpha}$  and  $E_2$ ), taxol and oestrone.
8. **Combinatorial Synthesis:** Principles, illustration with selected examples, advantages and limitations of combinatorial synthesis. Control measures for hazards in organic synthesis.
9. Control measures for hazards in organic synthesis.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Carry out different synthesis and transformation of the most common functional groups.
- (ii) Describe and apply stereochemical concepts such as chirality, stereoisomerism, and stereoselectivity in relation to chemical transformations.
- (iii) Identify, analyze and evaluate synthetic routes to target molecules by one-group and two group disconnections.
- (iv) Apply organometallic reagents and reactions in organic synthesis.
- (v) Plan and design experimental setups for various types of synthesis of biologically important organic compounds.

### Books Recommended

1. Stereoselective Synthesis in Organic Chemistry, Atta-ur-Rahman and Z. Shah.
2. Principles of Organic Synthesis, R. O. C. Norman.
3. Modern Synthetic Reactions, H. O. House.
4. Advanced Organic Chemistry: Reaction Mechanism and Structure, J. March.
5. Fundamentals of Organic Reaction Mechanisms, J. M. Harris and C. C. Wamser.
6. Reactive Molecules - The Neutral Reactive Intermediates in Organic Chemistry, C. Wentrup.

7. Organic Synthesis: The Disconnection Approach, S. Warren and P. Wyatt.
8. Advances in Heterocyclic Chemistry, S. F. Dyke.

## **ORG 526 Carbohydrates and Glycoconjugates**

**(3 Credits)**

### **Learning Objectives**

The learning objectives of this course are to

- (i) Give advanced knowledge on monosaccharides and their different structural features in different situations.
- (ii) Impart knowledge on synthesis of glycosides, anhydro-, amino-, and deoxy-sugars and their reactions.
- (iii) Have knowledge on the importance of polysaccharides and their industrial and biological importance.
- (iv) Acquire knowledge for isolation, purification and structural elucidation of complex polysaccharides.
- (v) Review the important polysaccharide derivatives and their applications.

### **Course Content**

1. **Configuration and Conformation:** Structure of monosaccharides and their stability in the form of furanose and pyranose.
2. **Structures and Shapes of:** Sugars of saturated five and six membered rings, acyclic carbohydrates, sugars in solution, mutarotation, anomeric ratio of furanoses and pyranoses, the influence of solvent and substitution.
3. **Reactions and Synthesis of:** Glycosides, Fischer glycosidation, amino-, deoxy-, anhydro- and thio- sugars, acidic cleavage of non-reducing sugars and their mechanism, Smith degradation, elimination, nitrous acids de-amination, selective oxidation, partial and enzymatic hydrolysis.
4. **The Biochemistry of Monosaccharides:** Catabolic or degradative reactions, interconversion of monosaccharides and synthesis of complex glycosyl compounds.
5. **A Comprehensive Study on:** Classification, isolation, purification, and structure elucidation of polysaccharides from plants, microorganism, algae and seaweeds, determination of linkage pattern of polysaccharides using spectroscopic and degradative methods.
6. **Dietary Fiber:** Soluble and insoluble dietary fiber; occurrence, linkage pattern and importance in protective different diseases.
7. **A General Study of Glycoconjugates:** Glyco-protein, proteoglycan, glyco-lipid and related compounds and their biological importance,

Glycosaminoglycans: Basic sugar residues of glycosaminoglycans; chitin, chondroitin-, heparin-, dermatan- and keratan sulfates.

8. **Isolation and Characterization of:** Bacterial *O*-antigen and their importance in developing vaccine against pathogenic microorganisms.
9. **Industrial Polysaccharides:** Structure, functions, and their large-scale production from plant sources and microorganisms.
10. **Cellulose Derivatives:** Carboxymethyl cellulose, cellulose acetates, sulphates etc., use of derivatives of cellulose in pharmaceutical and industrial purposes.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand the monosaccharide chemistry.
- (ii) Find out route to synthesize different monosaccharide derivatives.
- (iii) Understand the techniques of isolation and purification of complex polysaccharides..
- (iv) Elucidate the structure of complex polysaccharides using chemicals and spectroscopic means
- (v) Prepare industrially and biologically important polysaccharides derivatives and use them for suitable purposes.

### Books Recommended

1. Advanced in Carbohydrate Chemistry (Series).
2. Methods in Carbohydrates (Series).
3. Monosaccharides - Their Chemistry and Their Roles in Natural Products, P. M. Collins and R. J. Ferrier.
4. Polysaccharides, Vol. I-V, G. O. Aspinall.
5. Principles of Biochemistry, A. L. Lehninger.

## ORG 527 Natural Products

(3 Credits)

### Learning Objectives

The learning objectives of this course are to

- (i) Give basic knowledge on extraction, isolation & purification of natural products.
- (ii) Develop clear understanding of the chemistry of important natural products like terpenoids, alkaloids, steroids, hormones and natural pigments.
- (iii) Develop knowledge on biosynthesis of natural products.
- (iv) Have basic idea about natural products from marine sources

## Course Content

1. **Chemical Compounds in Living Species:** Synthesis and degradation through metabolism, biogenetic groupings of secondary metabolites and their role in chemiotaxonomic, classification of plants.
2. **Secondary Metabolism of Amino Acids and Cinnamic Acids:** Alkaloids derived from metabolism of ornithine, lysine, phenyl alanine, tyrosine, tryptophen, anthranillic acid, carbazoles, benzophenanthrine, protobarbarine and peptide derivatives, biogenesis of cinnamic acid derivatives, coumarines and its oxygenated derivatives.
3. **Secondary Metabolism and Ecology:** Plant-herbivore interaction, plant-insect interaction, plant-plant interaction and plant microorganism interaction.
4. **Chemical Characterization and Structural Elucidation of Secondary Metabolites:** Extraction with different solvents, isolation, purification through partition or adsorption process and detection of the chemical characterization by usual chemical methods and through chromatographic as well as different spectroscopic methods like UV, IR and NMR studies with the reference of alkaloids (morphine and reserpine), terpenoid (zinziberene and phytol), steroids (cholesterol, ergosterol) and hormones (testosterone, progesterone).
5. **Lipids:** Classification of lipids (simple, compounds and derived) and their biological functions such as glycolipids (phrenosin, kersin, nervone and hydroxynervone), phospholipids (lecithins, kephalins, plasmalogens and sphingomyelins), VLDL, LDL and HD, and their characteristics chemical reactions.
6. **Polypeptides and Proteins:** Chemical characterization and biological importance, elucidation of the secondary tertiary and quaternary structure of proteins, chemical composition and biological functions of insulin, glycoprotein, lipoprotein, chromoprotein and nucleoprotein.
7. **Nucleic Acids:** Chemical composition, classifications, biological functions and structural features of RNA and DNA by specific chemical reaction and spectroscopic methods, plant and animal viruses.
8. **Natural Dye and Pigments:** Natural dye and pigments, chemical composition and characteristics of natural dye and pigments with reference on indigotin, flavonoids and anthocyanins.

## Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Apply the extraction, isolation and purification techniques of different natural products like terpenoids and alkaloids.

- (ii) Demonstrate the steps of biosynthesis of carbohydrates, terpenoids alkaloids and steroids.
- (iii) Characterize different terpenoids, carotene flavonoids and alkaloids by chemical as well as spectroscopic methods.
- (iv) Explain the natural pigments like carotenoids, flavonoids etc.
- (v) Discuss the chemistry of different types of steroids, hormones steroidal alkaloids.

### Books Recommended

1. Organic Chemistry, Vol. 2: Stereochemistry and Chemistry of Natural Products, I. L. Finar.
2. Phytochemical Methods: A Guide to Modern Techniques of Plant Analysis, J. B. Harborne.
3. Secondary Metabolites, J. Mann.
4. Chemistry of Organic Natural Products, Vol. I and II, O. P. Agarwal.
5. Trease and Evans Pharmacognosy, W. C. Evans.
6. Organic Chemistry, F. A. Carey.

## ORG 528 Advanced Heterocyclic Compounds and Caged Hydrocarbons (3 Credits)

### Learning Objectives

The learning objectives of this course are to

- (i) Give the fundamental understanding of heterocyclic chemistry.
- (ii) Acquaint with the basic idea about structure, properties, synthesis and reactions of the important heterocyclic compounds, as well as different systems of nomenclature.
- (iii) Impart knowledge on the designing of synthetic routes for different heterocyclic compounds.
- (iv) Develop knowledge about preparation, properties and applications of caged hydrocarbons.

### Course Content

1. **Introduction:** Theoretical, synthetic, physiological and industrial significance of heterocyclic compounds, classification, systematic nomenclature.
2. **Compounds with Three-membered Heterocyclic Rings Containing Nitrogen, Oxygen and Sulphur:** Oxiranthiirans and aziridines - synthesis, physico-chemical properties, uses.
3. **Compounds with Four-membered Heterocyclic Rings Containing Nitrogen, Oxygen and Sulphur:** Oxetans, thietans and azetidines. Synthesis, physico-chemical properties, uses.

4. **Compounds Containing Five-membered Ring with Two Heteroatoms:** Synthesis, physico-chemical properties and uses of nitrogen-nitrogen (pyrazoles, imidazoles and related compounds), nitrogen-oxygen (oxazoles, isooxazoles and related compounds), nitrogen-sulphur (thiazoles, isothiazoles and related compounds) and nitrogen-selenium (selenazole compounds).
5. **Condensed Five-membered Rings with One Heteroatom:** Synthesis and physico-chemical properties of indoles, benzofurans, benzothiophenes and carbazoles.
6. **Compounds Containing Six-membered Ring with One Hetero Atom (Nitrogen, Oxygen and Sulphur):** Pyridine derivatives (alkyl and aryl pyridines, aminopyridines, halopyridines, hydroxypyridines, pyridine N-oxides, pyridine aldehydes and ketones), quinolines, isoquinolines, acridines and phenanthridines, pyrans and their derivatives (pyryliums and benzopyryliums, pyrans, benzopyrans, pyrones, benzopyrones), thiopyrans, thiochromenes and their derivatives.
7. **Compounds Containing Six-membered Ring with Two Hetero Atoms:** Pyridazines, pyrimidines, pyrazines, oxazines, thiazines, dioxanes, quinazolines, phthalazines, cinnolines and their analogues.
8. **Compounds Contain Seven-membered Rings:** Azepines, diazepines, oxazepines, thiazepines and related compounds.
9. **Synthesis of Some Biologically Important Heterocyclic Compounds:** Thiamine, nicotine, adenine, guanine, uracil, cytosine, quercetin, cyanidin, antipyrine, prontosil, sulphapyridine, barbituric acid, tryptophan, serotonin, folic acid.
10. **Saturated Heterocyclics with One and Two Hetero Atoms.**
11. **Adamantane and Related Polycyclic Systems.**
12. **Fullerenes.**

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand the importance of heterocyclic compounds in biological systems, pharmaceuticals and other industrial applications.
- (ii) Plan synthetic route of major classes of heterocyclic compounds.
- (iii) Demonstrate mechanisms for reactions involving heterocycles as starting materials, intermediates and products.
- (iv) Understand the preparation, properties and applications of caged hydrocarbons.

## Books Recommended

1. Chemistry of Carbon Compound (Heterocyclic Compounds), Vol. IV A, B, C ; E. H. Rodd.
2. Advances in Heterocyclic Chemistry, A. R. Katritzky.
3. The Chemistry of Heterocyclic Compounds, G. M. Badger.
4. Heterocyclic Chemistry, J. A. Joule, K. Mills and G. F. Smith.
5. The Principles of Heterocyclic Chemistry, M. Lagowski and A. R. Katritzky.
6. Heterocyclic Chemistry, R. K. Bansal.
7. An Introduction to the Chemistry of Heterocyclic Compounds. R. M. Acheson.
8. Heterocyclic Chemistry, T. L. Gilchrist.
9. Principles of Organic Synthesis, R. O. C. Norman.
10. The Chemistry of Heterocycles, T. Eicher, S. Hauptmann and A. Speicher.

## ORG 529 Organic Pollutants in the Environment

(3 Credits)

### Learning Objectives

The learning objectives of this course are to

- (i) Introduce general idea on common organic pollutants, their source, persistence and effects on living beings.
- (ii) Give general concept on toxicants and their doses, accumulation in organism and excretion.
- (iii) Impart knowledge on pollution by different hydrocarbons, industrial pollutants, organometallics, hazardous waste, fertilizers and their management.
- (iv) Acquaint with the pollution by traditional and modern pesticides, plant growth regulator and their formulation and various actions also food safety and poisoning.
- (v) Gain concepts on integrated pest management to reduce pollution.

### Course Content

1. **Introduction to Common Environmental Organic Pollutants and Their Sources:** Brief description about their persistence, log  $K_{ow}$ , bioaccumulation, biomagnification, biodegradation and biotransformation, persistent organic pollutants (POPs) and their effects on human and wild animals, a general overview about biosphere, atmosphere, anthrosphere, hydrosphere and geosphere.
2. **Toxicology:** Introduction to toxicology, dose-response relationship, dose and frequency of use, MRL (Maximum Recommended level) and (acceptable daily intake), routes and mechanism of entry of toxicants to organism, distribution of toxicants within the organism and

biotransformation, excretion, classes of poisons based on effect, quantitative principles of toxicology.

3. **Pollution by Hydrocarbons:** Occurrence, chemical nature, dispersion, evaporation, photooxidation and microbial transformation in the environment and aquatic organisms of petroleum, polycyclic aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs), hydroxylated PCBs (OH-PCBs), and dioxins, environmental distribution, persistency, toxicity, carcinogenicity of these compounds to human and wild life.
4. **Industrial Pollutants and Their Management:** Pollutants from Industries with special references to polymers and plastic, soap and detergents, pulp and paper, chemical and pharmaceutical industries, abatement procedures for the reduction of pollution from different industries.
5. **Organic Pollutants in Food Stuffs:** Pesticides (insecticides, herbicides and fungicides): classification, uses and effects on environment and human health with reference to traditional and modern pesticides, mechanism of action and metabolism of pesticides in biological system, detoxification and their metabolites in the environment, traditional pesticides: organochlorine (DDT, heptachlor, endosulfan, HCH, HCB), organobromine and organofluorine compounds, dirty dozens, Stockholm convention. Toxicology of HCB, DDT and its metabolites, modern pesticides: organophosphorous and organothiophosphorous (diazinon, malathion, chlorpyrifos, parathion, parathion-methyl), carbamic acid derivatives (carberyl, pirimicarb, etc.) phenoxy acid derivatives (2,4-D MCPA, MCPB, etc), MRL values and ADI of some common pesticides recommended by Codex Alimentarius Commission, United States Food and Drug Administration (USFDA) and World Health Organization (WHO), formulation of pesticides: Wettable powder, emulsion/solution and fumigants, etc., insect attractant, repellent and chemosterile retardants, plant growth regulators.
6. **Pollutants in Food:** Food safety, food poisoning, food-borne illness, contamination and hazard, symptoms of food poisoning, quality of foods, naturally occurring chemical contaminants: aflatoxin, isoflavones, saffrole, sinigrin, etc., artificial contaminants in food: synthetic food colors, dyes and pigments, preservatives, ripening agents, etc., harmful antibiotics in food: nitrofurans and its metabolites, chloramfenicol, etc.
7. **Organometallics Environmental Pollutants:** Nature, stability and sources of organometallic compounds, behavior in air, water, soil and sediments, organomercury, organolead, organotin and organoarsenic compounds.

8. **Pollution of Environment by Hazardous Waste Materials:** Nature, sources and environmental chemistry of hazardous wastes, hazardous wastes in atmosphere hydrosphere and biosphere, microbial metabolism in waste degradation, safe disposal by proper chemical and biological treatment of city waste, domestic and hospital wastes.
9. **Fertilizers:** Nitrogenous, phosphatic and NPK fertilizers, environmental implications of fertilizer; abatement procedure of fertilizer pollution.
10. **The Role of Integrated Pest Management to Control Pollution:** Integrated pest Management (IPM): Definition, Key components of IPM, Pest control techniques, Reduction of pollution. IPM in context of Bangladesh. biopesticides and use of biopesticides to produce organic agricultural products. Pest control by Pheromones. Use of pheromones in context of Bangladesh agriculture.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Demonstrate general idea on common organic pollutants, their source, persistence and effects on living beings.
- (ii) Apply general concept on toxicants and their doses.
- (iii) Manage various pollutions by different hydrocarbons, industrial pollutants, organometallics, hazardous waste, and fertilizers.
- (iv) Assess pollution by traditional and modern pesticides, their formulation also food poisoning and its safety.
- (v) Suggest integrated pest management plan to reduce pollution.

### Books Recommended

1. Basic Concept of Environmental Chemistry, D. W. Connell.
2. Fundamental Concept of Environmental Chemistry, G. S. Sodhi.
3. Organic Chemicals: An Environmental Perspective, A. H. Neilson.
4. Environmental Chemistry, A. K. De.
5. Environmental Pollution Analysis, S. M. Khopkar.
6. Environmental Chemistry: Air and Water Pollution, H. S. Stoker and S. L. Seager.
7. Environmental Chemistry, S. E. Manahan.
8. Handbook of Environmental Chemistry Series, O. Hutginger.
9. Environmental Toxicology, M. Stake, M. Mida, M. S. Sethi. S. A. Iqbal, H. Yasuhisa and S. Laguchi.

## ORG 530 Advanced Medicinal and Pharmaceutical Chemistry

(3 Credits)

### Learning Objectives

The learning objectives of this course are to

- (i) Give general aspects of the design & development of drugs including their classification, methods and routes of administration and production.
- (ii) Impart knowledge on structure-activity relationship (SAR), quantitative structure-activity relationship (QSAR), correlation of physicochemical properties, effect on drug action and pharmacokinetics.
- (iii) Explain drug action on nucleic acids, enzyme and proteins.
- (iv) Have knowledge on combinatorial synthesis for drug optimization and discovery.
- (v) Understand immunity, immunoglobulin, allergy, antihistaminic agents, antiviral agents, virus, cancer and anticancer agents.

### Course Content

1. **Introduction:** Fundamental aspects of drugs, classification of drugs, drug discovery and design, leads and analogues, methods and routes of drug administration, drug action, drug development and production.
2. **Chemical Structure-Activity Relationships in Drug Design:** Structure-activity relationship (SAR): Changing size and shape, introduction of new substituents, changing the existing substituents of a lead. Quantitative structure activity relationship (QSAR): Introduction, physicochemical properties, Hansch equation, the Craig plot, bioisosteres, and planning a QSAR study.
3. **Drugs Acting on Nucleic Acids:** Drugs that target nucleic acids (antimetabolites, enzyme inhibitors, intercalating agents, alkylating agents, antisense drugs, and chain-cleaving agents). Bacterial protein synthesis inhibitors.
4. **Drugs Action at Enzyme and Proteins:** Active sites and catalytic action, regulation of enzyme activity, mechanisms of action, enzyme inhibitors, drug design through enzyme inhibition, enzymes and drug resistance, drug action at carrier and structural proteins, protein and peptide drugs.
5. **Receptors and Messengers:** Introduction to receptors and messengers, receptor and the biological response, binding of ligands to receptors, ligand-receptor theories, receptor families, ion channels and their control, activation of membrane bound enzymes, neurotransmitters, neurotransmission processes, design of agonists and antagonists, partial agonists, depressants and stimulants.

6. **Combinatorial Synthesis for Drugs:** Principle of combinatorial synthesis, combinatorial synthesis for drug optimization and discovery, combinatorial synthesis in solid phase and solution phase.
7. **Immunobiologicals:** Cells of the immune system, immunity, acquisition of immunity, immunoglobulins, antigen-antibody reactions, vaccine.
8. **Allergy:** Introduction, histamine, allergens, storage and release of histamine, inhibition of histamine release, inhibition of released histamine, anti-histaminic agents, H<sub>1</sub> and H<sub>2</sub> antihistamines.
9. **Antiviral Agents:** Introduction, classification of virus, agents for the treatment of HIV infection, biochemical targets for antiviral therapy, infection process for a virus.
10. **Cancer and Cancer Chemotherapy:** Definition, principles, biochemical basis of cancer, type of cancers, cancer therapy, class of anticancer agents and their mechanism of actions.
11. **Pharmaceutical Chemistry:** Introduction, pharmacopoeias, types of analytical methods used for the determination of the purity of pharmaceutical substances, pharmacopoeial assay, example of some pharmacopoeial assays in relation to British Pharmacopoeia - aspirin, paracetamol, ascorbic acid, ampicillin, metronidazole.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand importance of chemistry in the development and application of therapeutic drugs.
- (ii) Relate the structure and physical properties of drugs to their pharmacological activity.
- (iii) Understand the physic-chemical properties of drugs.
- (iv) Understand the present drug development process and design new drug with the help of new scientific techniques.
- (v) Understand how changes in the chemical structure of drugs affect efficacy.
- (vi) Describe the overall process of drug discovery, and the role played by medicinal chemistry in this process.

### Books Recommended

1. Foye's Principles of Medicinal Chemistry, D. A. Williams and T. L. Lemke,
2. An introduction to Medicinal Chemistry, G. L. Patrick.
3. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, J. H. Block and J. M. Beale, Jr.
4. Medicinal Chemistry: An Introduction, G. Thomas.

5. Burger's Medicinal Chemistry and Drug Discovery, M. E. Wolff
6. Bentley and Driver's Textbook of Pharmaceutical Chemistry, L. M. Atherden.
7. Pharmacognosy, V. E. Tyler, L. R. Brady and J. E. Robbers.
8. British Pharmacopoeia Vol. I and II.

## **ORG 531 Food Chemistry and Technology**

**(3 Credits)**

### **Learning Objectives**

The learning objectives of this course are to

- (i) Acquire knowledge about nutritional value, taste, texture and freshness of food and food products.
- (ii) Understand food constituent and their interactions under different conditions.
- (iii) Find the methods to preserve and enhance availability and quality of food.
- (iv) Impart integral knowledge on the food science and technology.

### **Course Content**

1. **General Introduction:** Food, macro- and micro-nutrients in food, Digestion, absorption, metabolism.
2. **Carbohydrate:** Source of different types of starch and their consumption, glycemic index of starch. Dietary fiber (DF), importance of high and low DF content in staple food, addition of DF in bakery and other food products, cereals and their uses.
3. **Chemistry of Protein Occurs in:** fish meat, eggs, milk and milk products, lentils etc. and their nutritional values.
4. **Chemistry of Lipids:** Source, edible and non-edible fats/oils, their occurrence and consumption in food items. Free fatty acid,  $\omega$ -fatty acids, *trans*-fatty acids and their effects on human health.
5. **Sugars:** Plant sugar and artificial sweeteners (saccharine, cyclamate, sucralose, sorbitol, aspartame, dipeptide etc.) in food items.
6. **Food Additives:** Natural coloring agents, synthetic flavoring and coloring agents, and preservatives in foodstuff, isolation of lycopene from tomatoes, carotenes and tocopheroles, flavonoids and anthocyanins from vegetables.
7. **Toxicants:** Natural occurring toxicants in foods (anthocyanins, aflatoxins, safroles etc.), uses of medicinal plants in diet, synthetic toxicants in poultry meat, fish, soft drink, and other foodstuff.

8. **Genetically Modified Food:** Introduction, methodology and future prospect.
9. **Food Adulteration:** Adulteration in spice, oils and other foodstuff.
10. **Food Technology:** Constituents, Juice production from different fruits, production of vegetable and corn oils and their preservations.
11. **Food Additives and Food Preservatives:** Their chemistry, application and limitations.

### **Learning Outcomes**

Upon completion of this course, the students will be able to

- (i) Have general knowledge on food chemistry, such as carbohydrate, protein, lipids, etc.
- (ii) Gain in-depth knowledge on food additives, adulteration and food toxicants.
- (iii) Understand the general idea of genetically modified food and its future prospect.
- (iv) Understand modern food processing and preserving technology.

### **Books Recommended**

1. Food Chemistry, L. H. Meyer.
2. Chemistry of Food and Nutrition, H. C. Sherman.
3. Advanced Text Book on Food and Nutrition, Vol. I and II., M. Swaminathan,
4. Introductory Foods, M. Bennion and B. Scheule.
5. Food Science and Nutritional Health: An Introduction, T. P. Labuza and J. W. Erdman, Jr.
6. Food Science, H. Charley.
7. Foods and Food Production Encyclopedia, D. M. Considine and G. D. Considine.

## Detailed Syllabus for M.S. (Thesis Group) in Inorganic and Analytical Chemistry

### IA 541 Advanced Coordination Chemistry

(3 Credits)

#### Learning Objectives

The learning objectives of this course are to

- (i) Impart knowledge on molecular symmetry to predict molecular properties and provide hints about how the molecules change their symmetry when they take part in chemical reactions.
- (ii) Convey knowledge on different modern theories of bonding of coordination compounds.
- (iii) Express the structure and symmetries of coordination compounds with high coordination numbers and properties of cluster compounds.
- (iv) Discuss the origin of the electronic spectra of coordination compounds and their quantitative interpretation based on Orgel and Tanabe-Sugano diagrams.
- (ix) Convey knowledge of kinetics and reaction mechanism of coordination complexes.

#### Course Content

1. **Group Theory:** Symmetry analysis and its application, matrix representations of symmetry operations, characters and character tables, interpretation of character tables of chemically important symmetry groups, construction of molecular orbitals, symmetries of adopted orbitals, symmetries of molecular vibrations.
2. **An Overview of Theories of Bonding:** Valence bond theory, crystal field theory and its modification, molecular orbital theory for octahedral and tetrahedral complexes, a comparative study of these theories.
3. **Coordination Chemistry:** Structure and symmetries of complexes, molecular orbital model of  $ML_6$  and  $ML_4$  complexes, factors affecting the stability of complexes, metal ligand and metal-metal multiple bonds, complexes of high coordination numbers (higher than six) and their structural aspects.
4. **Spectra and Bonding of Complexes:** Russell Saunders couplings, microstates, ligand field spectra, selection rules and intensities, Orgel diagram in octahedral and tetrahedral fields, Tanabe Sugano diagrams and its applications, Nephelauxetic series, spectrochemical series, Jahn-Teller distortion and spectra, spectra of lanthanide and actinide complexes, spectra of M-M bonded complexes, charge transfer spectra, ligand to metal and metal to ligand charge transfer (LMCT and MLCT) transitions.

5. **Magnetic Properties:** Sources of paramagnetism, diamagnetism and Pascal's constants, magnetic properties based on crystal field model, determination of magnetic susceptibility by NMR method, anomalous magnetic moments, antiferromagnetism, ferromagnetism and ferrimagnetism, correlation of magnetic and structural properties.
6. **Reaction Mechanism of Transition Metal Complexes:** Electron transfer reactions, outer sphere and inner sphere reactions, two electron transfers reactions, synthesis of enantiomers and linkage isomers using electron transfer reaction, photochemical reactions, molecular rearrangements.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Discuss molecular symmetry and how symmetry helps us to understand molecular structure and many of a molecule's physical and chemical properties.
- (ii) Understand advanced theories of bonding of coordination compounds, their comparison and how these theories relate the structure and properties of transition metal complexes.
- (iii) Describe the electronic spectra of complex compounds and evaluate the crystal field splitting energy ( $\Delta_o$ ), inter-electronic repulsion parameters (A, B and C), etc. using Orgel and Tanabe-Sugano diagrams.
- (iv) Understand active metal sites of cluster compounds which are important for interaction with biological targets.
- (v) Investigate kinetics and mechanism of various types of reactions in coordination chemistry.

### Books Recommended

1. Advanced Inorganic Chemistry, F. A. Cotton G. Wilkinson, C. A. Murillo and M. Bochman.
2. Inorganic Chemistry, J. E. Huheey.
3. Inorganic Chemistry, G. L. Miessler and D. A. Tarr.
4. An Introduction to Inorganic Chemistry, K. F. Purcell and J. C. Kotz.
5. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford.
6. Chemical Applications of Group Theory, F. A. Cotton.
7. Infrared and Raman Spectra of Inorganic and Coordination Compounds, K. Nakamoto.
8. Mechanisms of Inorganic Reactions, F. Basolo and R. G. Pearson.
9. Inorganic Reaction Mechanisms, M. L. Tobe.

**Learning Objectives**

The learning objectives of this course are to

- (i) Impart knowledge about the class of compounds containing metal-carbon  $\sigma$  and  $\pi$  bonds, compounds with multiple metal-carbon bonds and their classification, naming system and application of 18e and 16e rule for  $\pi$ -donor complexes.
- (ii) Give knowledge on synthesis, structures and bonding of some main group and transition metal organometallic compounds and of metal clusters.
- (iii) Convey knowledge on the reactions of organometallic compounds and their mechanism such as insertion, oxidative addition, and reductive elimination etc.
- (iv) Impart knowledge on how these key reactions operate in various important catalytic processes.

**Course Content**

1. **General Features:** Nomenclature, classification of compounds with metal-carbon  $\sigma$  bond, compounds with metal-carbon  $\pi$  bond, compounds with multiple metal-carbon bonds, the 18e and 16e rule for  $\pi$ -donor complexes, back donation.
2. **Preparation, Structure and Bonding of Organometallic Compounds with Metal-Carbon  $\sigma$  Bond:** Metal alkyls and aryls, Grignard reagent, alkyl aluminums.
3. **Preparation Structure and Bonding of Organometallic Compounds with Metal-Carbon  $\pi$  Bond:** 2-electron donor e.g. Zeise's salt and other monoolefin complexes, 3-electron donor e.g.  $\pi$ -allyl and  $\pi$ -enyl complexes, 4-electron donor e.g. conjugated diolefin and cyclobutadiene complexes, 5-electron donor e.g. cyclopentadienyl complexes, 6-electron donor e.g. arene complexes, the isolobal analogy, agostic interaction.
4. **Properties of Metallocenes:** Aromaticity, basicity, magnetic susceptibility, ir spectra, electronic spectra and nmr spectra.
5. **Organometallic Reactions and Mechanisms:** Substitution reactions, insertion reactions: CO, SO<sub>2</sub> and olefin insertions, oxidative addition and reductive elimination reactions, ring expansion, ligand and metal exchange reactions.
6. **Catalytic Application of Organometallic Compounds:** Hydroformylation, hydrogenation of olefins, olefin metathesis, the Wacker process, dimerization of alkenes, polymerization of alkenes,

isomerization of alkenes, the 16- and 18-electron rule in homogeneous catalysis.

7. **Cluster:** Synthesis, structure and reactivity of osmium, ruthenium and iron clusters, copper cluster,  $\text{FeS}_4$ -cubane clusters and boron hydride cluster.
8. **Survey of Organometallic Compounds:** Chemistry of olefin and arene complexes.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Differentiate the organometallic and cluster compounds from other chemical compounds.
- (ii) Predict structures of organometallic and cluster compounds based on electron count rules.
- (iii) Designing of new compounds of this class and their reaction conditions.
- (iv) Understand the bonding of organometallic and cluster compounds.
- (v) Use organometallic and cluster compounds as catalyst for various commercial synthetic purposes.

### Books Recommended

1. Principles of Organometallic Chemistry, G. E. Coates, M. L. H. Green, P. Powell and K. Wede.
2. An Introduction to Organometallic Chemistry, A. W. Parkins and R. C. Poller.
3. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson.
4. Introduction to Cluster Chemistry, D. M. P. Mingos and D. I. Wales.
5. Organometallic Chemistry, P. L. Pausen.
6. Concepts and Models of Inorganic Chemistry, B. E. Douglas, D. H. McDaniel and J. J. Alexander.
7. Introduction to Metal  $\pi$ -Complex Chemistry, M. Tsutsui, M. N. Levy, A. Nakamura, M. Ichikawa and K. Mori.
8. Basic Organometallic Chemistry, B. D. Gupta and A. J. Elias.
9. Organometallic Chemistry, R. C. Mehrotra and A. Singh.
10. Inorganic Chemistry, G. L. Miessler and D. A. Tarr.
11. The Organometallic Chemistry of the Transition Metals, R. H. Crabtree.

### Learning Objectives

The learning objectives of this course are to

- (i) Impart knowledge on the structure and properties of different biomolecules and biomolecules incorporating metal ions.
- (ii) Acquaint the students with the techniques of isolation and purification of biomolecules and their characterization by physical and biochemical methods.
- (iii) Give concepts of beneficial and toxic effects of certain metals in certain forms and doses on life and how to detox heavy metals toxicity.
- (iv) Provide advance knowledge of the role of biological inorganic elements in electron transfer, oxygen transport, and other catalytic reactions in biological system.
- (v) Inform the biological roles of alkali and alkaline earth metals.

### Course Content

#### 1. Properties of Biological Molecules:

- (i) **Proteins and their constituents:** The naturally occurring amino acids and their properties, protein structure, protein as ligands.
- (ii) **Nucleic acids and their constituents:** RNA, DNA and their building blocks and properties, RNA structure, DNA structure, metal bonding and nucleic acid structure.
- (iii) **Other metal binding biomolecules:** Metalloproteins and metalloenzymes, coenzyme B<sub>12</sub>, prosthetic groups, oxygen carrying protein.

#### 2. Physical Methods in Bioinorganic Chemistry:

- (i) **Physicochemical methods:** NMR and Mössbauer spectroscopy, electrochemical methods, electron microprobe analyses.
- (ii) **Biochemical methods:** Measuring the molecular mass of a protein, measurement of macromolecule ligand binding affinities, protein isolation and purification.

#### 3. Control and Utilization of Metal-Ion Concentration: Beneficial and toxic effects of metal ions such as iron and zinc, toxic effects of mercury, arsenic, cadmium, lead, chromium and their detoxification.

#### 4. Bonding of Metal Ions and Complexes to Biomolecules: Selection and insertion of metal ions for proteins thermodynamic control, kinetic control, bioavailability, metal ion and metal complex binding to nucleic acids.

#### 5. Electron Transfer Proteins: Iron-sulfur proteins, cytochromes.

#### 6. Atoms and Group Transfer Chemistry: Dioxygen transport: hemoglobin and myoglobin, oxygen-atom-transfer reactions: Fe-

cytochrome, catechol and other dioxygenase, protective metalloenzymes - the Cu-Zn super oxide, dismutase.

**7. Biological Chemistry of Alkali and Alkaline Earth Metals:** Alkali metals and the regulation of membrane potentials, ion-pump.

**Learning Outcomes**

Upon completion of this course, the students will be able to

- (i) Describe the structure and functions of several biomolecules viz. proteins, DNA, RNA, etc. and of several metal binding biomolecules viz. metalloproteins, metalloenzymes, etc.
- (ii) Demonstrate fundamentals of advance physicochemical and biochemical methods used for structural characterization of biomolecules.
- (iii) Understand the beneficial role of some metal ions and toxic effects of heavy metals in biological system and their detoxification.
- (iv) Realize the kinetic and thermodynamic factors of binding metal ions with biomolecules leading to drug designing.
- (v) Appreciate the roles that metallic and nonmetallic elements play in biological systems to perform charge balance, electrolytic conductivity, signaling, electron transfer, group transfer, redox catalysis, energy storage, etc.

**Books Recommended**

1. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg.
2. Inorganic Biochemistry: An Introduction, J. A. Cowan.
3. Bioinorganic Chemistry, R. W. Hay.
4. The Biological Chemistry of the Elements - The Inorganic Chemistry of life, J. J. R. Fransto Da Silva and R. J. P. Williams.
5. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford.
6. Advanced Inorganic Chemistry, Gurdeep Raj, Vol. II.
7. Fundamentals of Biochemistry, J. I. Jain.
8. Text Book of Biochemistry; A. V. S. S. Rama Rao.

**IA 544 Inorganic Polymers and Macromolecules**

**(3 Credits)**

**Learning Objectives**

The learning objectives of this course are to

- (i) Acquaint the difference between inorganic and organic polymers.
- (ii) Explain the preparative method, structures and applications of some common inorganic polymers of boron, phosphorus, silicon, sulfur, etc.
- (iii) Discuss the structural and electronic features of metal complexes that lead to polymerization.

- (iv) Provide a fundamental knowledge about macromolecules, their structures, and functions in living organisms.
- (v) Convey knowledge on structures and functions of some common biomolecules.

## Course Content

1. **Inorganic Polymers:** General survey of inorganic polymers, classification and methods of study of inorganic polymers, comparison between inorganic and organic polymers.
2. **Classification, Preparation, Properties, Structural Aspects and Applications:**
  - (a) **Boron containing polymers:** (i) Boranes and (ii) borazines.
  - (b) **Phosphorus containing polymers:** (i) Polyphosphates, (ii) phosphonitrilic polymers (phosphazenes) and (iii) polyphosphazenes.
  - (c) **Silicon containing polymers:** (i) Silicones (fluid, elastomers and resins), (ii) silicates, (iii) polysilanes and (iv) polysiloxanes.
  - (d) **Sulfur-nitrogen polymers:** (i) Tetrasulfurtetranitride, (ii) trithiazyltrihalides, (iii) thiotrithiazyl cations, (iv) polythiazyl and (v) polythionic acids.
  - (e) **Carbon and fluorine containing polymers:** Fluorocarbons.
  - (f) **Metal-coordination polymers:** Preparation, classification, structures and uses.
  - (g) **Metal cluster systems.**
3. **Macromolecules:** The chelate and macrocyclic systems, types of ligands, macrocyclic amino ligands, aromatic amines, azadienes and related compounds, macrocyclic ligands and conjugated systems, phthalocyanines, Schiff's base ligands.
4. **Metallobiomolecules:** (i) Chlorophyll, (ii) vitamin B<sub>12</sub> and coenzyme B<sub>12</sub>, (iii) cytochrome C, (iv) nitrogenase, (v) PO<sub>4</sub> in biomolecules: ATP, DNA, RNA.

## Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Differentiate between organic and inorganic polymers.
- (ii) Assess appropriate method for the synthesis of a polymer and its structural characterization.
- (iii) Explore the exciting opportunities for their use as advanced materials for many different applications.
- (iv) Describe the basic units of the macromolecules and the types of linkages between them.
- (v) Understand the diversity and complexity of various biomolecules, their structures and properties.

## Books Recommended

1. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson.
2. Inorganic Chemistry, J. E. Huheey.
3. Chemistry of the Elements, N. N. Greenwood and A. Earnshaw.
4. Concepts and Models of Inorganic Chemistry, B. E. Douglas, D. H. McDaniel and J. J. Alexander.
5. Modern Aspects of Inorganic Chemistry, H. J. Emeleus and A. G. Sharpe.

## IA 545 Nuclear and Radiochemistry

(3 Credits)

### Learning Objectives

The learning objectives of this course are to

- (i) Impart advance knowledge on the different areas of nuclear chemistry including nuclear structure based on nuclear models, nuclear reactions and nuclear spectroscopy.
- (ii) Promote knowledge on nuclear technology, transuranium elements and hot atom chemistry.
- (iii) Describe how the electricity generated in a nuclear power plant.
- (iv) Discuss the health effects of radiation.
- (v) Inform the cosmic origin of the chemical elements.

### Course Content

1. **Nuclear Structure:** Models for nuclear structure and properties; optical model, Fermi-Dirac model, many particle shell model, collective model, comparisons of nuclear models, nuclear spin and statistics.
2. **Nuclear Spectroscopy and Instrumentation:**  $\alpha$ -,  $\beta$ -,  $\gamma$ -decay schemes,  $\beta$ - and  $\gamma$ -spectrometry, Mössbauer spectroscopy, high resolution  $\gamma$ -spectrometry with GE detectors,  $\alpha$ -spectrometry with silicon surface barrier detector, detection of neutrons with  $\text{BF}_3$  detectors.
3. **Transuranium Elements:** General ideas about transuranium elements ( $Z = 93-106$ ) and their nuclear properties, their production, separation and purification, their chemistry and uses.
4. **Hot Atom Chemistry:** Formation of recoil atoms, mechanism of reactions of recoil atoms, hot atom reactions in solids, reactions of recoil tritium and carbon atoms.
5. **Nuclear Technology and Energy:** Radiation induced chemical polymerization, surface curing of matters using  $\gamma$ -and UV-radiation, radiation chemistry of water, diagnostic and therapeutic uses of

radioisotopes ( $^{99}\text{Tc}$ ,  $^{125}\text{I}$ ,  $^{131}\text{I}$ ,  $^{68}\text{Ga}$ ,  $^{60}\text{Co}$ , etc.),  $\gamma$ -radiation for bone scanning, positron imaging, food preservation, generation of electrical energy from nuclear power stations, thermal and fast fission power reactors, fusion reactor technology.

6. **Nuclear Safety Issues:** Nature of environmental radioactivity and its transfer to the human body, biological effects of radiation- stochastic and non-stochastic effects, principles of environmental radiation-protection through personal monitoring, thermoluminescence dosimetry for natural radioactivity, radioactive wastes, recent methods to dispose critically dangerous radioactive wastes.
7. **The Origin of the Chemical Elements:** Cosmology - elemental abundances, cosmic abundance curves, stellar evolution: star populations, evolution of a star, stellar nucleosynthesis: hydrogen fusion, helium burning, the s-process, the r- and p-process, and supernovae.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand the nuclear structure come up by scientists with lots of different models, and principles of different detectors based on  $\alpha$ -,  $\beta$ -,  $\gamma$ -spectrometry.
- (ii) Elucidate the production, separation, purification and uses of transuranium elements.
- (iii) Understand the mechanism of reactions of recoil atoms and interpret the diagnostic and therapeutic uses of radioisotopes.
- (iv) Explain how radiation interacts with human tissues, what the possible consequences and the remedies are, and how to store and dispose of nuclear wastes.
- (v) Understand the fundamentals of the cosmic origin of the chemical elements and the nuclear history of the universe.

### Books Recommended

1. Radiochemistry and Nuclear Methods of Analysis, W. D. Ehmann and D. E. Vance.
2. Introductory Nuclear Physics, K. S. Krane.
3. Essentials of Nuclear Chemistry, H. J. Arnika.
4. Nuclear and Radiation Chemistry, B. K. Sharma.
5. Nuclear and Radiochemistry, G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller.

**Learning Objectives**

The learning objectives of this course are to

- (i) Introduce with crystalline and amorphous solids and the synthetic methods used and the new synthetic methods that have been developed to prepare pure and large single crystals.
- (ii) Impart knowledge on some aspects of crystal chemistry, crystal defects, and phase transition, properties like colour, magnetic, electrical conductivity, ferroelectricity, pyroelectricity, and piezoelectricity.
- (iii) Discuss the methods of characterization of crystalline solids, glasses, and ceramics and glass-ceramics materials.
- (iv) Promote knowledge on structure-property relationships, recent developments and technological applications of solid materials.
- (v) Provide the increasing knowledge of superconducting materials and their applications.

**Course Content**

1. **Introduction to Material Science:** Solids, classification of solids, theories of crystal structures, classification of structures, an overview of material science and recent developments.
2. **Synthesis of Solid Materials:** Reaction types, quality criteria and assessments, sol-gel technique, thin film preparation, chemical transport, thermodynamics of solid-state reactions, crystal growth, techniques of single crystal growth, liquid crystals, classification of liquid crystals and their possible phase transition, chemical structure of elements in liquid crystals, application of liquid crystals, solid solutions, requirements for solid solution formation, type of solid solutions.
3. **Properties of Solid Materials:**
  - (a) Ideal and defect structures of  $MX$ ,  $MX_2$ ,  $MX_3$ ,  $M_2X_3$ ,  $A_mB_nX_p$  type solids.
  - (b) Phase transitions, classifications of phase transition, stable and metastable phases, representations on phase diagrams.
  - (c) Conductivity, band structure of inorganic solids, dielectric materials, ferroelectricity, pyroelectricity, and piezoelectricity, application of ferropiezo and pyroelectrics.
  - (d) Color of inorganic solids.
  - (e) Structure and magnetic property relation of transition metal oxides, spinel, illmenites and perovskites.

#### 4. **Characterization of Solid Materials:**

- (a) **X-ray diffraction:** Structure determination from powder patterns, influence of crystal symmetry and multiplicities on powder pattern, limitation of powder methods.
- (b) **Neutron diffraction:** Neutron diffraction, applications, merits and limitation.
- (c) **Electron microscopy:** Electron diffraction applications, transmission electron diffraction applications, transmission electron microscopy (TEM), scanning electron microscopy (SEM), analytical electron microscopy (AEM).

#### 5. **Glasses and Ceramic Materials:** Different types of glasses and glass ceramics materials, fabrication and processing of glasses, ceramics phase diagrams, imperfection in ceramics, properties of glass and ceramics, natural and synthetic zeolites, application of zeolites.

#### 6. **Superconductors:** Superconductivity, theories of superconductivity, introduction of low $T_c$ and high $T_c$ superconducting materials, application, recent development of superconducting materials.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Describe various aspects or methods in solid state synthesis in greater detail.
- (ii) Understand the bonding and properties of solid materials.
- (iii) Explain the modern technology used to investigate the identification, chemical composition, structures of solid materials.
- (iv) Explain the mechanical, thermal, electrical properties of glasses, ceramics and zeolites.
- (v) Express recent developments of superconducting materials.

### Books Recommended

- 1. Solid State Chemistry and its Applications, A. R. West.
- 2. Solid State Chemistry-Techniques, A. K. Cheetham and P. Dey.
- 3. Introduction to Solid State Physics, C. Kittel.
- 4. Solid State Chemistry: An Introduction, L. E. Smart and E. A. Moore.
- 5. Basic Solid State Chemistry, A. R. West.
- 6. Materials Science and Engineering: An Introduction, W. D. Calister Jr.

## IA 547 Solution Chemistry

(3 Credits)

### Learning Objectives

The learning objectives of this course are to

- (i) Impart knowledge on some aspects of solvent systems and their properties.

- (ii) Promote knowledge on solutions, nature of solvents and their solvation properties, properties of solvated species.
- (iii) Discuss the environment and properties of metal ions into different solvent media.
- (iv) Convey the concept of solvated electron, properties and uses of solvated electron.

## Course Content

1. **Solvents and Solvation Numbers:** Solvents, classification of molecular solvents, general properties of ionizing solvents, hardness and softness in solvents, leaving effect of the solvent, solubility rules for salts, ions in solution, solvent numbers, determination of cation solvation number, secondary solvation and ion association, mixed solvents, behavior of mixed solvents, identification of mixed solvates.
2. **Aqueous Solution:** Types of reactions, distribution of aquo-cations, hydrolysis, acidity of hydrated cations, classification of cations by acidity category, pK values for aquo cations, oxo-aquo-cations, mixed aquo ligand complexes, mixed aqueous systems.
3. **Nonaqueous Solution:** Types of chemical reactions, measurement of solvent strength, study of some typical molecular nonaqueous solvents such as liquid ammonia, sulfuric acid, liquid sulfur dioxide, liquid hydrogen fluoride, liquid nitrogen tetroxide, bromine trifluoride, dimethyl sulfoxide, tetrahydrofuran, ethanol and molten salts.
4. **Properties of Metal Ion Solvation, Reaction Rates and Chemical Equilibria:** Enthalpies and free energies of formation of cations in solution, redox potentials of metal ions in solution, variation of redox potentials with cations, usefulness and limitations, reaction rates, factors affecting reaction rates, acid-base equilibria in aqueous solution, heterogeneous equilibria in aqueous systems.
5. **Methods of Investigation of Metal Ion Solvation:** Ionic conductances, entropies, viscosities, dielectric constants, refractivity, proton NMR, UV-visible, IR, ESR and Mössbauer spectroscopy.
6. **Solvated Electron:** Theoretical concept of solvated electrons, hydrated electron, reactions of the hydrated electron, the interconvertibility of  $e(aq)$  and  $H$ , hydrated electron scavengers, absorption spectrum, conductivity, and magnetic properties of metal ammonia solution, ammoniated electron, reactions of ammoniated electron, solvated electron in organic liquids.

## Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Differentiate between aqueous and nonaqueous solvents.

- (ii) Express the nature of different solvents, their properties, the solute-solvent interactions and its effect on many properties of the solute including solubility, reactivity and colour.
- (iii) Discuss the spectroscopic techniques (NMR, UV-visible, IR, ESR and Mössbauer spectroscopy) used for characterization of solvated metal ions and solvated electron.
- (iv) Explain the conductivity, entropies, dielectric constants, refractivity of solvated metal ions and solvated electrons.
- (v) Understand the reactions of solvated electrons in both aqueous and nonaqueous solutions.

### **Books Recommended**

1. Metal Ions in Solution, J. Burgess.
2. Ions in Aqueous Systems, T. Moeller and R. O'Connor.
3. Solvated Electron, Advances in Chemistry Series, R. F. Gould edited.

## **IA 548 Advanced Chemical Crystallography**

**(3 Credits)**

### **Learning Objectives**

The learning objectives of this course are to

- (i) Develop and extend knowledge on structural characterization of crystalline solids.
- (ii) Gain insights on diffractometry, single crystal, data collection, phase problem in crystallography, solution of the phase problem, refinement of the structure, and the results obtained.
- (iii) Give knowledge on electron density calculations using multipole refinement model.
- (iv) Impart an elementary idea on electron and neutron diffraction analysis of solids.

### **Course Content**

1. **X-rays and Crystals:** Diffractometry, choosing a crystal, crystal mounting, unique data, data collection, integrated intensities, the indexing of reflection and determination of space groups.
2. **Data Reduction and the Phase Problem:** Lorentz and polarization corrections, absorption and extinction corrections, radiation damage correction, scaling, unobserved reflections, temperature factors, the structure factor, Friedel's law, the Fourier transform, the electron density equation, the phase problem.
3. **Solution of the Phase Problem:** The Patterson function, Patterson symmetry, Harker lines, Harker planes, heavy atom method, direct methods: unitary structure factor, normalized structure factor, intensity

statistics, probability method, tangent formula, symbolic addition, modern developments.

4. **Completing the Structure:** Observed structure factor, calculated structure factor,  $F_o$  synthesis,  $\Delta F$  synthesis, identification of atom types, location of hydrogen.
5. **Refinement of Structures:** Matrix manipulations, the principles and practice of the method of least squares, series termination error, refinement by  $\Delta F$  synthesis, refinement against  $|F_o|^2$ , weighting function, goodness of fit parameter, residual indexes, restrained refinements.
6. **Derived Results:** Bond lengths, bond angles, and torsion angle calculations, calculation of esd's, correlation coefficients, thermal motions, anomalous scattering and its effects, absolute configurations.
7. **Electron Density:** Experimental electron density, promolecule density, deformation density, aspherical (multipole) refinement, merits of the multipole model.
8. **Electron and Neutron Diffraction:** Basic principles, applications and the limitations of these techniques.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Obtain specific competencies necessary for working in an educational institute as a crystallographer.
- (ii) Identify a single crystal, mounting it on a single crystal diffractometer, collect the data, reduce the data, solving the phase problem, complete and refine the structure, calculate the bond lengths, angles, torsion angles, etc.
- (iii) Demonstrate the important features of electron density map obtain from multiple refinement programs.
- (iv) Understand the principle of electron and neutron diffraction technique used for analysis of solids.

### Books Recommended

1. X-ray Structure Determination: A Practical Guide, G. H. Stout and L. H. Jensen.
2. Structure Determination by X-ray Crystallography, M. F. C. Ladd and R. A. Palmer.
3. Crystal Structure Analysis, J. P. Glusker and K. N. Trueblood.
4. Crystal Structure Analysis, M. J. Buerger.
5. Fundamentals of Crystallography, C. Giacovazzo, H. L. Monaco, D. Viterbo, F. Scordari, G. Gilli, G. Zanotti and M. Catti..

### Learning Objectives

The learning objectives of this course are to

- (i) Give a general understanding of working principle, instrumentation and applications of advanced analytical tools for surface characterization.
- (ii) Impart knowledge on working principle, instrumentation and applications of various advanced chromatographic techniques.
- (iii) Introduce knowledge on principle and types of electrophoretic techniques and scope of separation of low and high molecular weight charged materials including DNA, protein etc.
- (iv) Acquaint the students with the modern techniques used in ultratrace analysis; such as ICP-AES, ICP-OES, ICP-MS etc.
- (v) Give idea of automated methods in chemical analysis and computer based data processing.

### Course Content

1. **Surface Characterization by Spectroscopic and Microscopic Methods:** Spectroscopic methods: (i) ultraviolet photoelectron spectroscopy (UPS), (ii) metastable atom electron spectroscopy (MAES), (iii) X-ray photoelectron spectroscopy (XPS), (iv) X-ray fluorescence (XRF), (v) particle induced X-ray emission (PIXE), microscopic methods: atomic force microscopy (AFM), scanning electron microscopy (SEM) - principle, instrumentation and applications, baking technique in creating ultrahigh vacuum pressure.
2. **Chromatographic Techniques:** (i) GC-MS / LC-MS: Principles and investigation of toxic chemicals, (ii) ion and ion-pair chromatography: introduction and theory, columns and their packing, HPLC columns for ion chromatography, theory of ion-pair separation in liquid chromatography, use of ion pairing and ion suppression, effect of ionic strength and column temperature, normal and reversed phase ion-pair chromatography, (iii) size exclusion and supercritical fluid chromatography: theories of exclusion and supercritical chromatography, mechanism and materials, inorganic stationary phases, alkylated cross-linked dextrans, polyvinyl acetate gels, polystyrene-divinyl benzene gels, agars gels, (iv) properties of supercritical fluids, effect of pressure, stationary and mobile phases, optimization of separations, field-flow fractionation (FFF): principle of field-flow fractionation, separation mechanism, advantages of field-flow fractionation over chromatographic methods, detectors and applications in each technique.
3. **Electrophoretic Techniques:** Principle of electrophoresis, types of electrophoresis: scope of separation of low and high molecular weight

charged materials including DNA, protein, and enzymes etc. using electrophoretic techniques, sample introduction and detection.

4. **Techniques in Ultratrace Analysis:** (i) Inductively coupled plasma-atomic emission spectroscopy (ICP-AES), (ii) inductively coupled plasma-optical emission spectroscopy (ICP-OES), (iii) inductively coupled plasma-mass spectroscopy (ICP-MS): principle, instrumentation and applications including large scale metal analysis.
5. **Automated Methods in Chemical Analysis:** On-line flow injection analysis, data processing using softwares.

### **Learning Outcomes**

Upon completion of this course, the students will be able to

- (i) Discuss the spectra and images of target compounds through studying spectroscopic and microscopic techniques for the characterization of a surface.
- (ii) Apply various modern chromatographic techniques for the separation, identification and quantification using different detectors.
- (iii) Understand the mechanism of some ionization sources for mass spectrometry.
- (iv) Apply different electrophoretic and ultratrace analytical techniques.
- (v) Handle automated machine and computer based data processing for mass scale analysis.

### **Books Recommended**

1. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and T. A. Nieman.
2. Analytical Chemistry, G. D. Christian.
3. Modern Analytical Chemistry, D. Harvey.
4. Analytical Chemistry Handbook, J. A. Dean.
5. Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch.
6. Practical Liquid Chromatography, S. G. Parry, R. Amos and P. I. Brewer.
7. Analytical Chemistry Principles, J. H. Kennedy.
8. Chemical Analysis, H. A. Laitinen.
9. Instrumental Methods of Chemical Analysis, G. W. Ewing.
10. Modern Methods of Chemical Analysis, R. L. Pecsok and L. D. Shields.
11. Quantitative Chemical Analysis, D. C. Harris.

### Learning Objectives

The learning objectives of this course are to

- (i) Discuss some basic principles of modern electroanalytical techniques.
- (ii) Impart knowledge on various electrochemical cells and electrodes.
- (iii) Give knowledge on pulsing techniques in controlled potential electrolysis and their application for analytical purposes.
- (iv) Impart knowledge on various electroanalytical techniques such as amperometric titration methods, coulometry, chronopotentiometry, spectroelectrochemistry, electrochemical sensors and their applications.

### Course Content

1. **Review of Some Basic Electroanalytical Processes:** Redox process, mass transport and diffusion process and charge transfer reactions at the electrode surface, advanced polarographic techniques.
2. **Electrochemical Cells and Electrodes:** (a) Types of cells: three electrode electrochemical cells, (b) electrodes of new generations: hanging mercury drop electrode (HMDE), rotation microdisk electrode (RMDE), mercury film electrode (MFE), Hg and Au film electrodes on glassy carbon, carbon paste electrode, graphite electrodes, chemically modified electrodes, enzyme electrodes, microfibre electrodes: carbon, gold and platinum fibre electrodes.
3. **Pulsing Techniques in Controlled Potential Electrolysis:** Normal pulse, differential pulse and square wave pulse and their analytical use and advantages compared to direct current-voltage measurements.
4. **Pulse Voltammetry and Stripping Voltammetric Analysis:** (i) Differential pulse and square-wave pulse voltammetry for inorganic trace analysis, (ii) anodic and cathodic stripping analysis with differential and square wave pulse techniques for trace analysis and chemical speciation studies, (iii) adsorptive stripping voltammetry for ultra trace-electroanalysis, applications of electroanalysis in inorganic and organic compounds.
5. **Amperometric Titration Methods:** Principle, electrode titration procedure, successive titration, advantages and disadvantages of amperometry, applications.
6. **Coulometry:** Principle, variation in coulometric technique, coulometry at controlled potential, coulometry at constant current, secondary coulometric titration, advantages and disadvantages, applications.
7. **Chronopotentiometry and Spectroelectrochemistry:** Principle and application.

- 8. Electrochemical Sensors:** (i) Ion sensors for specific environmental applications, (ii) gas-sensing ions selective electrodes, and (iii) potentiometric biosensors for biochemical analysis.

### **Learning Outcomes**

Upon completion of this course, the students will be able to

- (i) Demonstrate the knowledge of different types of cells and various types of electrodes of new generation.
- (ii) Apply different pulsing techniques in controlled potential electrolysis and their application for analytical purposes.
- (iii) Use different pulse voltammetry and stripping voltametric techniques for analysis of inorganic and organic compounds.
- (iv) Obtain specific competencies on various electroanalytical techniques such as amperometric titration methods, coulometry, chronopotentiometry and spectroelectrochemistry and electrochemical sensors and their applications.
- (v) Serve in an educational or research institute as an electrochemist.

### **Books Recommended**

1. Analytical Chemistry, G. D. Christian.
2. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and T. A. Nieman.
3. Analytical Electrochemistry, J. Wang.
4. Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch.
5. Electrochemical Methods, A. J. Bard and L. R. Faulkner.
6. Organic Electrochemistry, An introduction and a Guide, H. Lund and M. M. Baizer.

## **IA 551 Environmental Monitoring and Analysis**

**(3 Credits)**

### **Learning Objectives**

The learning objectives of this course are to

- (i) Demonstrate a general idea on environmental pollution, need for environmental monitoring and socioeconomic benefits of pollution control.
- (ii) Impart knowledge on water quality parameters determination, wastewater treatment and management of different polluted water systems.
- (iii) Acquaint students with the detailed knowledge about atmospheric composition, monitoring of various pollutants in the atmosphere using modern analytical techniques, their effects such as global warming, climate change etc.

- (iv) Give knowledge on analysis of biological material and genobiotics, basic principle and methodology of bio-monitoring in pollution effects study and application of biotechnology in pollution control
- (v) Introduce knowledge on quality control of processed food and beverages.

## Course Content

### 1. Basic Principle and Need for Environmental Monitoring and

**Analysis:** Occurrence of pollution episode, temporal and spatial variation of pollutants, Sampling and analytical planning, method selection, quality control and quality assurance, calibration and validation, errors, contribution of different errors to quality control, limit of detection, interpretation of analytical data, documentations, development of standard operating procedures (SOP), socioeconomic benefits of pollution control, regulatory compliance with control measures, guidelines for policy intervention, and technical solution to an environmental problem.

### 2. Analysis of Water and Wastewater:

Aquatic environment, water pollutants, water quality parameters and standards, sampling and preservation, general aspect of chemical analysis of water pollutants, analytical methods (spectrophotometric, electrochemical, chromatographic, and mass spectroscopic), analysis of water samples, automated water analysis, eutrophication, waste water treatment, management of river pollution, ground water formation, aquifer, lifetime and hydrological studies of ground water pollution and their characteristic studies (environmental geochemistry): stable environmental isotopes (H, D, T,  $^3\text{He}$ ,  $^{12}\text{C}$ ,  $^{13}\text{C}$ ,  $^{16}\text{O}$ ,  $^{18}\text{O}$ ), arsenic contamination in ground water.

### 3. Ambient Air and Trace Gases Analysis:

Composition and structure of the atmosphere, earth radiation balance, atmospheric sampling and monitoring, particles, ions, and radicals in the atmosphere, photochemical reactions in the atmosphere, greenhouse gases and global warming, ozone hole and climate change, analysis of gases (sulphur dioxide, nitrogen oxides, carbon monoxide), FTIR and LIDAR system for remote sensing of gaseous air pollutants, determination of hydrocarbon and organics (VOCs, NHHCs), particulate matters (SPM,  $\text{PM}_{10}$  and  $\text{PM}_{2.5}$ ), high and low volume samplers, impactors, size distributions, chemical composition, analysis of black carbon, organic carbon, air toxic substances like POPs, PAHs, etc., trace metals analysis (iron, copper, lead, mercury, etc.), ground level ozone monitoring (chemiluminescence and UV spectroscopic method), trend analysis, air quality index (AQI).

4. **Analysis of Biological Material and Xenobiotics:** Xenobiotics, indication of exposures to xenobiotics, determination of metals, nanometals, inorganic and organic compounds, measurements of different phase reaction products, determination of adducts, and promise of immunological methods.
5. **Biomonitoring and Environmental Impact Analysis:** Bio-monitoring: basic principles and methodology of biomonitoring, bioindicators, bioassay techniques in pollution effects study, application of biotechnology in pollution control: bioinformatics, biotechnology and pollution control, bioremediation, biosensors and its application, biological deodorisation, biological purification of contaminated air, environmental impact analysis (EIA): principle, characteristics of the environmental problem, origin of the environmental pollutants and their chemical nature, distribution of pollutants in environmental compounds around the sources, assessment of impact on water bodies and biota.
6. **Monitoring of Processed Food and Beverages:** Quality control analysis of processed food and beverages for both inorganic and organic contaminants, for examples, soft drinks, Jam Jelly.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Demonstrate about environmental pollution and needs of its monitoring.
- (ii) Treat wastewater and manage different water systems.
- (iii) Determine various pollutants in the atmosphere and demonstrate their adverse effect on the globe.
- (iv) Apply different bio-monitoring methodology in pollution effects study and apply bio-technology in pollution control.
- (v) Find out the quality of processed food such as soft drink, Jam Jelly etc.

### Book Recommended

1. Environmental Chemistry, S. E. Manahan.
2. Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch.
3. Modern Analytical Chemistry, D. Harvey.
4. Air Chemistry, T. Godish and J. S. Fu.
5. Environmental Chemistry, P. O'Neil.
6. Environmental Chemistry, A. K. De.
7. A Textbook of Environmental Chemistry and Pollution Control, S. S. Dara and S. Chand.
8. Food Contaminants: Origin, Propagation and Analysis, S. N. Mahindru.

**Learning Objectives**

The learning objectives of this course are to

- (i) Discuss the biotic and abiotic components of an ecosystem and describe the interactions between these components.
- (ii) Impart advance knowledge on water pollution, air pollution, marine pollution, toxicology chemistry and marine chemistry.
- (iii) Promote knowledge on water treatment, solid waste management and management of aquatic environment.
- (iv) Discuss the guidelines for healthy environment.

**Course Content**

- 1. Introduction to Aquatic and Biotic Pollutants.**
- 2. Water Pollution:** Nature and types of water pollutants, elemental pollutants, heavy metals, metalloids, organically bound-metals and metalloids, inorganic species, algal nutrients and eutrophication, organic pollutants-pesticides in water, polychlorinated biphenyls (PCBs), poly-aromatic hydrocarbons (PAHs), radionuclides in the aquatic environment, pollutants from agriculture in aquatic environment (fertilizers).
- 3. Water Treatment:** Preliminary treatment, screening, skimming, primary treatment, sedimentation, flocculation, activated sludge method, oxidation ponds, sludge disposal, tertiary treatment, chlorination, wet oxidation, adsorption, reverse osmosis, electrodialysis, ion exchange, fluoridation, drawbacks of chlorine disinfection method, ultraviolet (UV) disinfection treatment.
- 4. Humic Substances in the Aquatic Environment:** Physico-chemical characteristics of human substances in water and soil, complexation reactions of humic and fulvic acids with metal ions, detoxification of toxicants through the formation of complexes, ions of some specific examples.
- 5. Toxicological Chemistry in the Environment:** Toxicants in the environment, impact of toxic chemicals on enzymes, biochemical effects: As, Cd, Pb, Hg, CO, nitrogen oxides, sulfur oxides, ozone and cyanides, pesticides, environmental fate of toxicants, health risk, assessment of toxicants.
- 6. Management of Solid Waste:** Classification of solid wastes, disposal of bulk solid wastes, organic waste, direct disposal of animal wastes on land, composting, sewage sludge, biogas from solid wastes, mixed urban wastes, land filling, incineration, recycling and reuse.

7. **Management of Aquatic Environment:** Water quality and human health, development of charter to ensure its quality for designated use, environment impact assessment (EIA) of water pollution on aquatic lives and food quality, environmental laws and regulations to control discharge of liquid and solid wastes into water bodies, national environment quality standards (EQS), EEC and WHO guidelines for environmental health criteria, the earth summit.
8. **Marine Chemistry and Marine Resources:** Basic concepts in marine chemistry, solubility and carbonate and bicarbonate equilibria of alkali earth metals in seawater and marine sediments, sea fishes, sea foods, phytoplankton, oil and gases, metals, nonmetals and minerals.
9. **Marine Pollution:** Classification of marine pollutants, inorganics; Cd, Cu, Pb, Hg, organics; insecticides, polychlorinated biphenyls (PCBs), polyaromatic hydrocarbons (PAHs), polycyclic aromatic hydrocarbons (PCAHs), dioxins, radioactive materials, oil pollution and its effects on biota, abatement of marine pollution.
10. **Atmospheric Pollution and Its Effects:** Natural air pollution, anthropogenic air pollution, gas phase pollutants and photochemical smog formation, visibility, turbidity, thermal air pollution, atmospheric deposition, acid rain, stratospheric ozone depletion, global warming, health effects: air pollution episodes, pollution exposures, impact of pollutants on human health, health effects of respiratory air particles and PAN, health effects of noise pollution.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Identify the types of air and water pollutants and deal with the various water treatment processes.
- (ii) Explore the importance of humic substances in the aquatic environment and understand the marine chemistry, importance of marine resources and marine pollution.
- (iii) Identify the toxic chemicals in the environment and their detrimental effects on human health
- (iv) Manage different aquatic environment free of pollution and manage different types of solid wastes.
- (v) Understand the safety recommendation and regulations of water and air pollution for maintaining healthy environment.

### Books Recommended

1. Environmental Chemistry, G. W. Vanloon and S. J. Dufty.
2. Air Quality, T. Godish, W. T. Davis and J. S. Fu.
3. The Chemistry of Pollution, G. Fellenberg.

4. Atmospheric Chemistry, B. J. Finlayson-Pitts and J. N. Finlayson-Pitts.
5. Environmental Chemistry, S. E. Manahan.
6. Fundamental Concept of Environmental Chemistry, G. S. Sodhi.
7. Environmental Chemistry, A. K. De.
8. Environmental Toxicology, M. Satake, Y. Mido, M. S. Sethi and S. A. Iqbal.
9. Environmental Hazards, K. Smith.
10. Environmental Analytical Chemistry, F. W. Fifield and E. J. Haines.
11. Minerals from the Marine Environment, Sir P. Kent.
12. Marine Geo-Chemistry, R. Chester and U. Hyman.
13. Application of Environmental Chemistry, E. R. Weiner.
14. Toxic Metal Chemistry in Marine Environments, M. Sadiq.
15. Environmental Chemistry: Air and Water Pollution, H. S. Stoker and S. L. Seager.

## **Detailed Syllabus for M.S. (General Group) in Chemistry**

### **Theoretical Course**

The detailed learning objectives, course content and learning outcomes of theoretical courses to be taken by the students for M.S. degree in Chemistry (non-thesis group) are given in the detailed syllabus of three different branches of chemistry.

### **Laboratory Course**

#### **PC 515 Physical and Environmental Chemistry Laboratory (3 Credits)**

#### **Learning Objectives**

The learning objectives of this course are to

- (i) Acquaint with the practical knowledge of measurement or study of light intensity, physicochemical behavior of binary liquid system, mixed surfactant systems etc.
- (ii) Familiarize with techniques for the electrochemical study of redox active substances and treatment of wastewater.
- (iii) Give practical training for studying kinetics of catalyzed reactions and adsorption on solid-liquid interfaces.
- (iv) Impart knowledge on destruction of waste textile dyes, phenomena related to photochemical reactions and estimation of air pollutants.
- (v) Acquaint with the technique of nano-particles preparation and their characterization.

#### **Course Content**

1. Determination of intensity of light by chemical actinometry and determination of quantum yield of some photochemical reactions.
2. Investigation of kinetics of some reactions catalyzed by micelles.
3. Electrochemical study of redox active substances.
4. Treatment of waste water from textile and tannery industries by electrocoagulation.
5. Study of the physicochemical properties of a binary liquid mixture.
6. Quantum chemical calculation on chemical bonding and intermolecular forces.
7. Kinetics of adsorption on solid-liquid interfaces and determination of thermodynamic parameters.
8. Surface phase behavior in mixed surfactant systems.

9. Mineralization of textile dyes by Fenton/photo-Fenton processes.
10. Preparation of nano particles and their characterization.
11. Investigation of pollutants in the air.

### Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Measure or study of light intensity, phenomena related to photochemical reactions, physicochemical behaviour of binary liquid system, mixed surfactant systems etc.
- (ii) Apply electrochemical techniques for studying redox couples and waste water treatment.
- (iii) Demonstrate kinetics of catalyzed reactions and adsorption phenomena on solid-liquid interfaces.
- (iv) Degrade waste textile dyes from aqueous solution using photochemical reactions and estimate air pollutants.
- (v) Prepare and characterize nano-particles.

### Books Recommended

1. Practical Physical Chemistry, A. Findlay.
2. Practical Physical Chemistry, S. R. Palit.
3. An Introduction of Practical Chemistry, K. K. Sharma.
4. Recent Reports in the Relevant Field.

## ORG 535 Organic Chemistry Laboratory

(3 Credits)

### Learning Objectives

The learning objectives of this course are to

- (i) Provide practical knowledge in the multistep synthesis and quantitative estimation by chemical, spectroscopic and chromatographic techniques.
- (ii) Impart practical knowledge on separation of the mixture of compounds by selecting suitable chromatographic techniques.
- (iii) Acquaint with the extraction of volatile components from plant by steam distillation.

### Course Content

1. Study of the Kinetic versus thermodynamically controlled reaction.
2. Solvolyses of alkyl halides.
3. Conversion of maleic acid to fumaric acid and vice versa.
4. Preparation of modified starch to be used in textile finishing.
5. Determination of  $\alpha$ -cellulose content in cotton.

6. Determination of protein content in food sample.
7. Determination as well as identification of saturated and unsaturated fatty acids in food samples.
8. Identification of essential and non-essential amino acids in leafy and non-leafy vegetables by paper chromatography using ninhydrin spray.
9. Detection of the types of phytochemicals in the organic solvents and aqueous extractives of plant samples including medicinal plants.
10. Multi-step organic synthesis of pharmaceutically important compounds.
11. Isolation of coloured pigments from different food stuff.
12. Investigation of natural and synthetic polymer.
13. Isolation of casein from milk.
14. Preparation of liquid glucose from starch.

### **Learning Outcomes**

Upon completion of this course, the student will be able to

- (i) Prepare liquid glucose, modified starch, pharmaceutically important compounds using multi steps and convert one compound to other and vice versa.
- (ii) Study kinetics of a reaction.
- (iii) Identify essential and non-essential amino acids, phytochemicals and saturated and unsaturated fatty acids in different samples.
- (iv) Determine  $\alpha$ -cellulose, protein content, saturated and unsaturated fatty acids etc.
- (v) Apply isolation techniques for the isolation of coloured pigments from food stuff, casein from milk etc.

### **Books Recommended**

1. A Text Book of Practical Organic Chemistry, A. I. Vogel.
2. Comprehensive Practical Organic Chemistry, V. K. Ahluwalia and S. Dhingra.
3. Preparative Methods of Polymer Chemistry, W. R. Sorenson and T. W. Campbell.

## **IA 555 Inorganic and Analytical Chemistry Laboratory (3 Credits)**

### **Learning Objectives**

The learning objectives of this course are to

- (i) Demonstrate knowledge of preparing a Schiff's base, metal complexes of Schiff's base and of other ligands and their characterization.

- (ii) Offer the chance of gaining practical experience of analyzing various environmental samples by spectrophotometric method.
- (iii) Impart practical knowledge on separation and quantification by anion exchanger, paper and thin layer chromatography.
- (iv) Give knowledge on the determination of composition and stability constant of complexes.
- (v) Demonstrate the techniques of preparation and characterization of ternary metal oxide, nonstoichiometric compounds and geopolymers etc.

## Course Content

Requisite numbers of experiment are to be chosen from the following list of experiments.

1. Preparation of Schiff's base metal complexes and their characterization.
2. Analysis of chromium(VI) from environmental samples by UV-visible spectrophotometric method.
3. Separation of zinc and magnesium on an anion exchanger.
4. Separation of cadmium and zinc on an anion exchanger.
5. Determination of chromium and manganese simultaneously by using spectrophotometric method.
6. Preparation and characterization of ternary metal oxides.
7. Solid state synthesis of nonstoichiometric compounds.
8. Synthesis and characterization of geopolymer.
9. Separation of bromophenol blue, congo red, phenol red mixture using thin layer chromatographic technique.
10. Determination of the purity of urea produced from natural gas.
11. Determination phosphate from environmental samples.
12. Separation and identification of metal ions by paper and thin layer chromatography.
13. Analysis of natural waters for pH, total hardness, phosphate, sulphate and oxygen.
14. Analysis of arsenic from environmental samples by using UV-visible spectrophotometric method.
15. Determination of composition of complex ion  $[\text{Ni}(\text{en})_n]^{2+}$  by Job's continuous variation method.
16. Determination of stability constant of  $[\text{Ni}(\text{glycinate})_n]^{(2-n)+}$ .

17. Preparation and resolution of  $[\text{Co}(\text{en})_3]^{3+}$ .
18. Preparation and characterization of  $[\text{Co}(\text{NH}_3)_4\text{CO}_3]\text{NO}_3$  and  $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$ .

### Learning Outcomes

Upon completion of this course, the students will be able to

- (ii) Design new ligand, prepare new complexes and adopt different techniques for their characterization.
- (iii) Analyze various environmental samples by spectrophotometric method.
- (iv) Separate, identify and quantify various metal ions by using different separation techniques.
- (v) Prepare and characterize ternary metal oxide, nonstoichiometric compounds and geopolymers etc.
- (vi) Identify and solve chemical problems and explore new areas of research.

### Books Recommended

1. A Textbook of Quantitative Inorganic Analysis, A. I. Vogel.
2. Practical Inorganic Chemistry: Preparations, Reactions and Instrumental Methods, G. Pass and H. Sutcliffe.