



**SMIT** SIKKIM  
MANIPAL  
UNIVERSITY  
SIKKIM MANIPAL INSTITUTE OF TECHNOLOGY

**M.Sc. Chemistry Syllabus Revision-2025**  
**M.Sc. 1 year Chemistry**  
**M.Sc. 2 years Chemistry**



**DEPARTMENT OF CHEMISTRY**  
**SIKKIM MANIPAL INSTITUTE OF TECHNOLOGY**  
**MAJHITAR, RANGPO, EAST - SIKKIM, INDIA**

## SIKKIM MANIPAL UNIVERSITY

### VISION:

- Global Leadership in Human Development, Excellence in Education and Healthcare.

### MISSION:

- Develop professionals of excellent technical calibre in the field of Health Sciences, Engineering, Management and Social Sciences with a humane approach capable of shouldering the responsibility of building the nation and be globally competent.

### OBJECTIVE:

- To support, promote and undertake the advancement of academics.
- To promote use of ICT and modern education technologies.
- To encourage research, creation and dissemination of knowledge.
- To facilitate extension and community service.
- To empower people of Sikkim and contribute to human development in Northeast.
- To create environmental and social responsibilities among students and employees.
- To ensure steady growth of the University.

## SIKKIM MANIPAL INSTITUTE OF TECHNOLOGY

### VISION:

- To achieve eminence in the field of quality technological education and research.

### MISSION:

- To develop SMIT into an Institution of Excellence capable of producing competent techno-managers who can contribute effectively to the advancement of the society.

### OBJECTIVE:

- To provide wholesome education to meet the intellectual aspirations of the students.
- To equip students with techno-managerial skills to enable them to take their assigned role in the industry.
- To inculcate essential ethics and values to meet the spiritual needs to the students.
- To provide a sound institutional environment nurturing emotional strength, healthy mind, body and resilience amongst the students.

## DEPARTMENT OF CHEMISTRY

### VISION:

- To emerge as a centre of excellence in teaching and research.

### MISSION:

- To equip the students with latest knowledge in science and technology such as to contribute as valuable members of the society.

### OBJECTIVE:

- To provide quality teaching and research.
- Inculcate societal responsibility in the students.
- To provide sufficient training in terms of latest developments in the field of chemistry.

### PO's

1. Develop and refine fundamental knowledge of Chemistry.
2. Cultivate in –depth knowledge in Organic chemistry, Inorganic chemistry, Physical chemistry, Analytical chemistry and Spectroscopy.
3. To improve analytical and logical capability to import the ability to solve new and complex problems.
4. Developing the teamwork philosophy.
5. Imbibing research acumen and innovative thinking to become a good researcher.
6. Motivating and developing the knack for clearing competitive exams.
7. Developing presentation skill and improving / fine tuning personal interaction.
8. To use the knowledge for the betterment of the society.
9. Acquire hands on experience in experimental chemistry.

### PSO

1. To develop up-to-date knowledge in different fields of chemistry.
2. Ability to carry out challenging research work in the frontier areas.

### PEO

1. To motivate and prepare post graduate students through effective coaching for higher education and research.
2. To impart education and training to the students for better employment.

**Department of Chemistry**  
**Proceedings of Board of Studies Meeting conducted on 29<sup>th</sup> May/4<sup>th</sup> June 2025**  
**at Room No: A-301 of Chemistry, SMIT at 03.00 PM**

The following members were present:

1. Dr. Satadru Jha, Chairperson, BOS, Department of Chemistry
2. Prof. (Dr.) Sangeeta Jha, Internal Member, BOS, Department of Chemistry.
3. Dr. Manoranjan Pandey, Internal Member, BOS, Department of Chemistry.
4. Dr. Ramesh Sharma, Internal Member, BOS, Department of Chemistry.
5. Dr. Santanu Gupta, Internal Member, BOS, Department of Chemistry.
6. Dr. Moazzam Ali, Internal Member, BOS, Department of Chemistry.
7. Prof. (Dr.) Prasenjit Maity, School of Engineering and Technology, National Forensic sciences University, Guwahati– External Expert BOS.
8. Dr. Tabrez Khan, Associate Professor, School of Basic Sciences, IIT- Bhubaneswar, External Expert, BOS.
9. Dr. Gautam Patel, Deputy General Manager, Medicinal Chemistry, Zydus Ahmedabad, Gujarat, External Expert, BOS.
10. Dr. Parita Basnet, Assistant Professor, Dept. of Chemistry, Sikkim Institute of Science and Technology Chisopani, Namchi – Alumni Expert, BOS.

**Agenda:** The Board met for syllabus revision of the following:

1. M.Sc. 1 year Chemistry
2. M.Sc. 2 years Chemistry

**Resolution:**

- i) There is a major revision (more than 20%) in the syllabus of M.Sc. 1 year and 2 years program for continuous improvement in cutting edge progress era.
- ii) To build up research interest among students a 4 credit Dissertations is incorporated in the II<sup>nd</sup> semester M.Sc. 2 years program.
- iii) The total credit of M.Sc. program remains same as earlier i.e. 85.
- iv) The syllabus of each course is divided into 5 Modules and each module carry one CO.
- v) The subject codes are changed as per university policy.
- vi) The Summary of modification are given as Annexure I.
- vii) Detailed modification of M.Sc. 1 year and 2 years program is carried out and given as Annexure 363II.

Dr. Satadru Jha  
Chairman/HOD Chemistry  
SMIT, Sikkim

Prof. (Dr.) Sangeeta Jha  
Internal Members  
Department of Chemistry  
SMIT, Sikkim

Prof. (Dr.) Prasenjit Maity  
External Expert  
School of E&T  
NFSU, Guwahati

Dr. Tabrez Khan  
External Expert  
School of Basic Sciences  
IIT-Bhubaneswar  
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Dr. Gautam Patel  
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Medicinal Chemistry  
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Dr. Manoranjan Pandey  
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Dr. Ramesh Sharma  
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Dr. Moazzam Ali  
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Dr. Parita Basnet  
External Member  
Sikkim Institute of Science and Technology  
Namchi, Sikkim

## ANNEXURE 1

**M.Sc. Chemistry Curriculum**  
**M.Sc. Chemistry: 1 year (43 Credits)**  
**M.Sc. Chemistry: 2 years (85 Credits)**

<b>DEPARTMENT OF CHEMISTRY</b>			
<b>Curriculum for 1 yr M.Sc. Chemistry w.e.f. 2025-27</b>			
<b>M.Sc. (CHEMISTRY) 1<sup>st</sup> Semester</b>			
1.	CH601B1	Advanced Coordination Chemistry & Inorganic Reaction Mechanism	4
2.	CH602B1	Concepts in Organic Synthesis	4
3.	CH603B1	Chemical Dynamics and Electrochemistry	4
4.	EL-I	Elective I (special paper)	4
5.	CH601B4	Inorganic Chemistry Lab	3
6.	CH602B4	Organic Chemistry Lab	3
7.	CH601B5	Project Based Learning	1
<b>Total Credit of semester I</b>			<b>23</b>
<b>M.Sc. (CHEMISTRY) 2<sup>nd</sup> Semester</b>			
1.	CH604B1	Bio-inorganic Chemistry	3
2.	CH605B1	Solid State Chemistry and Interface Science	3
3.	CH606B1	Group Theory – A Chemist Approach	3
4.	CH607B1	Quantum Chemistry- II	3
5.	EL-II	Elective II (Special Paper)	4
6.	CH601B6	Research Project Work	4
<b>Total Credit of semester II</b>			<b>20</b>
<b>ELECTIVE I</b>			
1.	CH601B3	Photoinorganic Chemistry	4
2.	CH602B3	Synthetic Organic Chemistry	4
3.	CH603B3	Advanced Physical Chemistry	4
<b>ELECTIVE II</b>			
1.	CH604B3	Chemistry of Nanomaterials	4
2.	CH605B3	Supramolecular Chemistry	4
3.	CH606B3	Medicinal Chemistry	4
<b>M.Sc. Chemistry Total Credit</b>			<b>43</b>

<b>DEPARTMENT OF CHEMISTRY</b>			
<b>Curriculum for 2 yrs M.Sc. Chemistry w.e.f. 2025-27</b>			
<b>M.Sc. (CHEMISTRY) 1<sup>st</sup> Semester</b>			
<b>Sl. No.</b>	<b>Sub Code</b>	<b>Sub Name</b>	<b>Credit</b>
1.	CH501B1	Principles of Inorganic Chemistry	4
2.	CH502B1	Principles of Organic Chemistry	4
3.	CH503B1	Chemical Thermodynamics	4
4.	CH504B1	Analytical Chemistry	4
5.	CH501B4	Physical Chemistry Lab	3
6.	CH502B4	Analytical Chemistry Lab	3
		<b>Total Credit of semester I</b>	<b>22</b>
<b>M.Sc. (CHEMISTRY) 2<sup>nd</sup> Semester</b>			
1.	CH505B1	Modern Spectroscopic Technique	4
2.	CH506B1	Organic Reactions and Mechanisms	4
3.	CH507B1	Biochemistry	4
4.	CH508B1	Quantum Chemistry- I	4
5.	CH505B6	Dissertation (6 months)	4
		<b>Total Credit of semester II</b>	<b>20</b>
<b>M.Sc. (CHEMISTRY) 3<sup>rd</sup> Semester</b>			
1.	CH601B1	Advanced Coordination Chemistry & Inorganic Reaction Mechanism	4
2.	CH602B1	Concepts in Organic Synthesis	4
3.	CH603B1	Chemical Dynamics and Electrochemistry	4
4.	EL-I	Elective I (special paper)	4
5.	CH601B4	Inorganic Chemistry Lab	3
6.	CH602B4	Organic Chemistry Lab	3
7.	CH601B5	Project Based Learning	1
		<b>Total Credit of semester III</b>	<b>23</b>
<b>M.Sc. (CHEMISTRY) 4<sup>th</sup> Semester</b>			
1.	CH604B1	Bio-inorganic Chemistry	3
2.	CH605B1	Solid State Chemistry and Interface Science	3
3.	CH606B1	Group Theory – A Chemist Approach	3
4.	CH607B1	Quantum Chemistry- II	3
5.	EL-II	Elective II (Special Paper)	4
6.	CH602B6	Research Project Work	4
		<b>Total Credit of semester IV</b>	<b>20</b>

<b>ELECTIVE I</b>			
1.	CH601B3	Photoinorganic Chemistry	4
2.	CH602B3	Synthetic Organic Chemistry	4
3.	CH603B3	Advanced Physical Chemistry	4
<b>ELECTIVE II</b>			
1.	CH604B3	Chemistry of Nanomaterials	4
2.	CH605B3	Supramolecular Chemistry	4
3.	CH606B3	Medicinal Chemistry	4
<b>M.Sc. Chemistry Total Credit</b>			<b>85</b>

# **ANNEXURE II**

# **Syllabus for M.Sc. 1-year Program**

**M.Sc. Chemistry - Semester I (M.Sc. 1-year Program)**  
**Advanced Coordination Chemistry & Inorganic Reaction Mechanism**  
**Subject Code: CH601B1**

**(Credits: Theory-04)**

**Course Objectives**

Detailed understanding of CFT, LFT & MOT and their use in inorganic complexes. Understanding of various types of transitions and their interpretation. Introduction to reaction mechanism with examples. Understanding of special organometallic reactions

**Course/Learning Outcome:** At the end of the course, the students will be able to:

CO1: Understanding of VBT, CFT, CFSE and their applications. Influence on distortion of spectra.

CO2: Understanding fundamentals of molecular orbital theory and ligand field theory.

CO3: Ability to predict electronic transitions and interpret electronic spectra of transition metal complexes.

CO4: Understanding fundamentals of reaction mechanism & electron transfer reaction mechanism.

CO5: Understand the importance of use of organometallic catalysts in different reactions & bonding in carbonyl complexes.

**Module I**

**Nature of Metal Ligand Bonding in Complex Compounds** (10 Lectures)

Valence bond theory in octahedral, tetrahedral & square planar complexes, Crystal field theory (CFT), Splitting of d orbital in octahedral, Tetrahedral and square planar complex, Crystal Field Stabilization Energy (CFSE), Determination of  $\Delta_o$  (CFSE) for various configurations, factors influence the magnitude of  $\Delta_o$ , application of CFT, Jahn-Teller Distortion.

**Module II**

**Molecular Orbital Theory & Ligand Field Theory** (10 Lectures)

Molecular Orbital Theory (MOT), Molecular orbital approach to bonding in octahedral complexes, Energy order of orbitals and their filling with electrons, sigma bonding in octahedral and tetrahedral complexes,  $\pi$  bonding in octahedral complexes,  $\pi$  donor ligands (CTLM),  $\pi$  acceptor ligands (CTML), Orgel diagram, Tanabe-Sugano diagram, Ligand field theory, Nephelauxetic effect, evidence for covalent bonding in complexes: adsorption spectra and Electron paramagnetic resonance spectra. (EPR).

**Module III**

**Electronic Spectra of Transition Metal Complexes** (10 Lectures)

Microstate calculation, L-S coupling, coupling of orbital angular momenta, coupling of spin angular momenta, selection rule, calculation of ground state terms, Hund's rule, Mulliken symbol in octahedral field, Orgel diagram, Spectra of  $d^1$  and  $d^9$ ,  $d^2$  and  $d^8$ ,  $d^3$  and  $d^7$  in octahedral & tetrahedral complex,  $d^5$  and  $d^8$  spectra in octahedral complex. Microstate table and its use in predicting electronic transitions.

**Module IV**

**Inorganic Reaction Mechanism** (09 Lectures)

Substitution and electron transfer reaction - Nucleophilic Substitution in square planar and octahedral complexes, Kinetics, Associative - Dissociative mechanisms, Trans effect, influence of acids-bases and other factors in reactions. Outer sphere and Inner sphere electron transfer in

octahedral complexes, electron transfer and its application, kinetic and thermodynamic stability, Labile and inert complexes.

### **Module V**

#### **Special Organometallics & Bonding in Carbonyl Complexes** (09 Lectures)

Bonding in Carbonyl complexes, Special organometallics - Reaction and applications, Suzuki reactions, Stille reaction, Negishi Cross coupling, Heck reactions, Buchwald-Hartwig reaction, Sonogashira reaction.

#### **Textbooks/Reference Books**

1. Advanced Inorganic Chemistry - F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann.
2. Inorganic Chemistry, Principles of Structure and Reactivity - James E. Huheey, Ellen A. Keiter, Richard L. Keiter.
3. Inorganic Chemistry - Atkins and Shriver.
4. Inorganic Chemistry – G. L. Miessler, P. J. Fischer & D. A. Tarr.

**M.Sc. Chemistry - Semester I (M.Sc. 1-year Program)**  
**Concepts in Organic Synthesis**  
**Subject Code: CH602B1**

**(Credits: Theory-04)**

**Course Objective**

This course will introduce the basic idea of Pericyclic reactions, Organic photochemistry, concepts of oxidation-reduction, heterocyclic chemistry and introduction of natural products.

**Course/Learning Outcome:**

CO1: Ability to identify and deduce mechanisms of various types of pericyclic and photochemical reactions.

CO2: In-depth understanding of solid-state chemistry of peptides and its applications.

CO3: In-depth understanding of catalysis in chemistry and its applications.

CO4: Ability to identify and apply oxidation-reduction reactions in synthesis.

CO5: In-depth knowledge of heterocyclic chemistry and its applications.

**Module I**

**Pericyclic Reactions**

(09 Lectures)

Postulates and derivation of the kinetic gas equation; collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity, calculation of  $\sigma$  from  $\eta$ ; variation of viscosity with temperature and pressure. Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy.

**Module II**

**Organic Photochemistry**

(08 Lectures)

Principle, photochemical energy, orbital symmetry consideration related photochemical reactions, electronic oxidation, excited state of organic molecule, modes of dissipation of energy, energy transfer, quantum yield, cis-trans isomerization, photo-fragmentation reaction (Barton, Hofmann-Löffler-Freytag), Norrish type (I) & (II) reactions, Paterno Buchi reaction, Photo reduction, di-pi methane, aza-di-pi methane rearrangement, photocyclo addition, Photo chemistry of  $\alpha$ ,  $\beta$ -unsaturated ketones, reaction with singlet oxygen, application of photochemical methods in organic synthesis (Tranylcypromine).

**Module - III**

**Oxidation & Reduction Reactions**

(08+07 Lectures)

**Reduction:** Reduction of C-C multiple bond and carbon-hetero multiple bond: Catalytic hydrogenation (both hydrogen and hydride transfer mechanism), Electrochemical reduction at a low overvoltage electrode, Reduction by metal hydrides and alkoxides (LAH, DIBAL-H,  $\text{Bu}_3\text{SnH}$ ), Borane and borohydride,  $\text{R}_3\text{SiH}$ , Reduction by dissolving metals, Stereo/enantioselectivity reductions (Chiral Boranes, Corey-Bakshi-Shibata).

**Oxidation:** Formation of C=C by dehydrogenation – dehydrogenation by selenium dioxide, Formation of alcohols from hydrocarbons, Jones reagent, Sarett's reagent, PCC, Swern oxidation,

MnO<sub>2</sub>, IBX, MPV, Pb(OAc)<sub>4</sub>, NaIO<sub>4</sub>, HIO<sub>4</sub>, Dakin reaction, O<sub>3</sub>, *m*-CPBA, VO(acac)<sub>2</sub>, Sharpless asymmetric epoxidation.

#### Module - IV

##### Heterocyclic Chemistry (07 Lectures)

Introduction, classification, nomenclature, reactions of aziridine, oxirane, thiirane, oxaziridine, azetidine, azetidinone, oxetane, oxetanone, thietane, pyrrole, furan, thiophene, 1,2- and 1,3-azoles, triazoles, pyridine, diazines, triazine and their oxy-derivatives. Application of heterocycles in various emerging fields - especially in medicine, and natural products.

#### Module - V

##### Catalysis (06 Lectures)

Heterogeneous catalysis: Preparation of catalyst and applications heterogeneous catalysis in synthesis of drugs. Homogenous catalysis: Introduction, hydrogenation, Wilkinson catalysts, Ziegler-Natta catalysts, applications of homogeneous catalysis in synthesis of drugs.

##### Chemistry of Peptides (03 Lectures)

Principle and methods of solid phase peptide synthesis, activation procedures, coupling reactions, protection, deprotection and cleavage from resin.

#### Textbooks/Reference Books

1. Finar, I. L., Organic Chemistry, vol. I & II (ELBS).
2. Advanced Organic Chemistry by J. March, Wiley Interscience.
3. Organic Chemistry by Morrison and Boyd
4. Reaction mechanism in organic chemistry by Mukhreji & Singh
5. Design of organic synthesis by M. Taylor
6. Stereochemistry of Carbon Compounds – E. L. Eliel
7. Organic Chemistry – J. Clayden; N. Greeves; S. Warren; P. Wothers
8. Modern Methods in Organic Synthesis – W. Carruthers

**M.Sc. Chemistry - Semester I (M.Sc. 1-year Program)**  
**Chemical Dynamics and Electrochemistry**  
**Subject Code: CH603B1**

**(Credits: Theory- 04)**

**Course Objectives**

The objective behind studying Chemical dynamics and electrochemistry is to present theories and applications related to the various chemical reactions and also to update the students with the latest developments in the above field.

**Course/Learning Outcomes (CO):**

CO1: To impart basic knowledge of Chemical Kinetics of Collision theory and the activated complex theory. To understand the mechanisms of unimolecular reactions.

CO2: To understand the chemistry of Complex reactions, consecutive reactions, chain reactions, oscillatory, Thermal & photochemical chain reactions. To understand the kinetics of fast reactions.

CO3: To acquire knowledge on electrolytic conductance and the principles of Debye-Huckel model of ion-ion interactions and its verification.

CO4: To understand the theory of Activity and activity coefficients in electrolytic solutions.

CO5: To impart knowledge on electrified interface and Approximate models of electrified interface.

**Module I**

**Chemical Kinetics-I**

(12 Lectures)

Arrhenius equations, concept of transition state, transition state theory-mechanism, collision theory, steric factor, comparison between collision & Transition state theory, Potential energy surface, thermodynamic treatment of reaction rates, Energy of activation, volume of activation, Series & Parallel reactions, Equilibrium from kinetic point of view, Kinetic isotope effect and solvent isotope effect, treatment of unimolecular reactions-Lindemann's theory, Hinshelwood's theory.

**Module II**

**Chemical Kinetics-II**

(10 Lectures)

Complex reactions, consecutive reactions, chain reactions and oscillatory, Thermal & photochemical chain reaction between  $H_2$  &  $Cl_2$  and  $H_2$  &  $Br_2$ , Influence of dielectric constant and ionic strength on reaction rate, linear free energy relationship, effect of substituents, fast reactions. Luminescence and energy transfer process, study by stop flow techniques, relaxation method.

**Module III**

**Electrochemistry**

(08 Lectures)

Electrolytic Conductance- Theory of electrolytic conductance: Degree of dissociation, time of relaxation, Mechanism of electrolytic conductance. Dispersion of conductance: Debye-Falkenhagen effect and Wien effect. Onsager equation, Debye – Huckel theory of dilute electrolytes, derivation of Debye-Huckel conductance equations for dilute solution, Verification of Debye – Huckel theory.

## Module IV

### Free Energy and Activity

(10 Lectures)

Activity & activity coefficients, its method of determination, Forms of activity coefficients and significance. Significance of the Degree of Dissociation- ion-pairs and factors affecting ion pair formation. Activities of Electrolytes and Values of Activity Coefficients. Limiting & extended Debye-Huckel equation for activity coefficient, The Huckel and Bronsted Equations.

## Module V

### Electrified Interface

(08 Lectures)

Approximate models of electrified interface: Helmholtz Compact layer model, Gouy-Chapman diffuse layer model and Stern Model.

### Textbooks/Reference Books

1. Laidler, K. J. Chemical Kinetics 3rd Ed., Pearsons (2011)
2. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006)
3. McQuarrie, D. A. & Simon, J. D. Physical Chemistry: A Molecular Approach 3rd Ed., Univ. Science Books (2001)
4. Bockris, J. O' M. & Reddy, A. K. N. Modern Electrochemistry 1: Ionics 2nd Ed., Springer (1998).
5. Bockris, J. O' M. & Reddy, A. K. N. Modern Electrochemistry 2B: Electrodictics in Chemistry, Engineering, Biology and Environmental Science 2nd Ed., Springer (2001)
6. Bockris, J. O' M., Reddy, A. K. N. & Gamboa-Aldeco, M. E. Modern Electrochemistry 2A: Fundamentals of Electrodictics 2nd Ed., Springer (2001).
7. Brett, C. M. A. & Brett, A. M. O. Electrochemistry, Oxford University Press (1993)
8. Moore, W. J. Physical Chemistry 4th Ed. Prentice-Hall (1972).
9. Electrochemistry, S. Glasstone

**M.Sc. Chemistry - Semester I (M.Sc. 1-year Program)**  
**Photoinorganic Chemistry**  
**Subject Code: CH601B3**

**(Credits: Theory- 04)**

**Course Objective**

Introduction to photochemistry, concepts, application and industrial use.

**Course/Learning Outcome**

CO1: In- depth understanding of photochemical Laws, Ability to explain various photophysical process taking place in excited state and factors influencing them.

CO2: Ability to identify and explain photophysical kinetics of excited state in gaseous and liquid state and electron transfer process.

CO3: In-depth understanding of photo-reduction and related reactions.

CO4: Ability to identify various types of photochemical reactions and its application.

CO5: In-depth understanding of photochemical reactions in biological processes and its explanation using model systems.

**Module I**

**Introduction to Inorganic Photochemistry** (10 Lectures)

Importance of photochemistry, Laws of photochemistry, quantum yield, thermochemical and photochemical reactions, photochemical equilibrium, photochemistry and spectroscopy, Charge transfer and charge transfer to solvent transition. Photophysical process in electronically excited molecules - Jablonski diagram, radiation-less transitions, selection rules. Fluorescence emission, fluorescence and structure. Triplet states and phosphorescence emission.

**Module II**

**Collisions in Solution & Kinetics** (10 Lectures)

Photophysical kinetics of unimolecular process, delayed fluorescence, effect of temperature on emission processes. Photophysical kinetics of bimolecular process – kinetic and optical collisions, bimolecular collisions in gases and vapours. collisions in solution, kinetics of collisional quenching: Stern-Volmer equation, deviations, Excimer and excited state dimers, exciplex formation and decay. electronic energy transfer mechanism.

**Module III**

**Photo Reduction and Related Reactions** (10 Lectures)

Photo reduction and related reactions, Photo oxidation and photo oxygenation, Chemiluminescence, Photosensitization. Photochemical reactions; substitution, decomposition and fragmentation, rearrangement, and redox reactions.

**Module IV**

**Photochemical Reaction** (09 Lectures)

Photochemical reaction between anthracene and carbon tetrachloride, determinations of quantum yield of reaction, factors affecting the quantum yield of reaction, Photoreactive state of anthracene.

## Module V

### Selective Inorganic Photochemistry

(09 Lectures)

Selective inorganic photochemistry using laser beams. Inorganic photochemistry in biological processes and their model studies- Mutagenic effect of radiation, Photosynthesis.

### Texts Books/Reference Books

1. Organometallic Photochemistry, Academic Press, 1979 – G.L. Geoffrey & M. S. Wrighton
2. Fundamentals of Photochemistry, Wiley Eastern, 1978 – K. K. Rohatagi-Mukherjee
3. Inorganic and Organometallic photochemistry, ACS Pub., 1978 – M. S. Wriphron
4. Photochemistry of Co-ordination compounds, Academic Press, 1970 – V. Balzani and V. Carassiti

**M.Sc. Chemistry - Semester I (M.Sc. 1-year Program)**  
**Synthetic Organic Chemistry**  
**Subject Code: CH602B3**

**(Credits: Theory- 04)**

**Course Objective**

This course will discuss the use of various organometallic compounds in organic synthesis, chemistry of B, P, S. Moreover, the role of transition metal complexes in organic synthesis and asymmetric synthesis will be covered in this subject area. Knowledge on retrosynthesis, protection & deprotection of functional group and application of spectroscopy for the determination of organic structures will be provided to make clear understanding among students about organic synthesis.

**Course/Learning Outcome**

CO1: Explain and identify organometallic and their uses in organic synthesis.

CO2: Explain and identify organometalloid and their uses in organic synthesis.

CO3: Ability to demonstrate knowledge of asymmetric synthesis.

CO4: Design retro-synthetic strategies independently for compounds of moderate complexity.

CO5: Explain and solve how to project and deprotect functional groups during organic synthesis.

**Module I**

**Organometallics of Group I & II and Organometalloids**

(16 Lectures)

Organometallic compound of Gr I and II metals: preparation and properties, reaction with carbonyl and alkylating agents.

Boron Chemistry: Organoboranes- preparation and properties of organoborane reagents e.g.  $\text{RBH}_2$ ,  $\text{R}_2\text{BH}$ ,  $\text{R}_3\text{B}$ , 9-BBN, Thexyl borane, cyclohexyl borane, Hydroboration-mechanism, stereo and regioselectivity, uses in synthesis of primary, secondary tertiary alcohols, aldehydes, ketones, alkenes. Synthesis of E, E; E, Z; Z, Z dienes and alkynes. Allyl boranes- synthesis, mechanism and uses.

Phosphorous Chemistry: Preparation & properties of  $\text{PPh}_3$ ,  $\text{P}(\text{OEt})_3$ ,  $\text{POCl}_3$ ,  $\text{PBr}_3$ ,  $\text{PCl}_5$ , etc. Wittig-Horner reaction, Mitsunobu reaction, Staudinger reaction, Vilsmeier-Haack reaction, Corey-Winter reaction.

Sulphur Chemistry: Reaction with  $\text{CS}_2$ ,  $\text{SO}_2$ ,  $\text{SO}_3$ ,  $\text{SOCl}_2$ ,  $\text{SO}_2\text{Cl}_2$ ,  $\text{PhSNa}$ , 1,3-dithiane, DMSO,  $\text{RSCl}$ , sulphur ylide in organic synthesis.

**Module II**

**Transitional Metals Complexes in Organic Synthesis**

(10 Lectures)

Introduction, oxidation states of transition metals, 16-18 rule, dissociation, association, insertion, oxidative addition, reductive elimination of transition metal.

Organocopper Intermediates: Preparation and structure, reaction involving organocopper.

Organopalladium in Organic Synthesis: Heck arylation, allylic activation, carbonylation, wacker oxidation, isomerization formation N-aryl and N-alkyl bond transmetalation.

Organonickels: Coupling carboxylation, carbonylation. Reaction involving rhodium and ruthenium.

### Module III

#### Asymmetric Synthesis (10 Lectures)

Stereoselective and stereospecific reactions, prochirality, Chemo-, regio-, diastereo- and enantio-controlled approaches; Chirality transfer, Asymmetric inductions; Chiral pools, Chiral auxiliaries, Chiral reagents and catalysts, and templates.

Asymmetric Oxidations: dihydroxylation, aminohydroxylation, Asymmetric reduction reactions: Reduction of ketones, imines and olefins (use of BINAP).

Asymmetric C-C Bond Forming Reaction: Simmons-Smith reaction, Mukaiyama aldol reaction, Shibasaki bi-metallic catalyst system.

### Module IV

#### Retrosynthesis (06 Lectures)

Basic principles and terminology of retrosynthesis, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions.

### Module V

#### Protection & Deprotection of Functional Group (06 Lectures)

Protecting Groups: Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection; illustration of protection and deprotection in synthesis.

#### Texts Books/Reference Books

1. Advanced Organic Chemistry by J. March, Wiley Interscience.
2. Organic Chemistry by J. Clayden; N. Greeves; S. Warren; P. Wothers
3. Principles of Organic Synthesis by R. O. C. Norman
4. Modern methods in organic synthesis organic synthesis by W. Carruthers and I. Coldham
5. Advanced Organic Chemistry - Part B: Reactions & Synthesis by F. A. Carey & R. J. Sundberg
6. Chiron approach in organic synthesis by S. Hanessian (Relevant chapters for Chirons)
7. Asymmetric Reactions and Processes in Chemistry: Ernest L. Eliel
8. Comprehensive Organic Transformations: A Guide to Functional Group Preparations, 2nd edition (1999) by Richard C. Larock.
9. Protective Groups in Organic Synthesis, 3rd edition (1999) by Theodora W. Greene and Peter G. M. Wuts

**M.Sc. Chemistry - Semester I (M.Sc. 1-year Program)**  
**Advanced Physical Chemistry**  
**Subject Code: CH603B3**

**(Credits: Theory- 04)**

**Course Objective**

To introduce the concepts of statistical mechanics and thermodynamics as it relates the macroscopic properties of a system to the properties of the atoms and molecules which constitutes a system.

**Course/Learning Outcome**

CO1: Able to find the connection between statistics and thermodynamics. and differentiate between classical statistics and quantum statistics.

CO2: Able to account for the physical interpretation of partition functions and be able to calculate thermodynamic properties of model systems with using Boltzmann, Fermi-Dirac and Bose-Einstein statistics

CO3: Ability to understand basics of Quantum Statistics.

CO4: Able to understand process of aggregation of amphiphilic molecules and their industrial application.

CO5: Ability to determine surfactant aggregation using experimental techniques.

**Module I**

**Statistical Thermodynamics** (10 Lectures)

Basic Statistical Thermodynamic, Phase space, Assembly & Ensemble, canonical form, statistical equilibrium & thermodynamic probability, Maxwell Boltzmann statistics.

**Module II**

**Partition Function** (10 Lectures)

Partition function and its types – Translational, Rotational, Vibrational, and Electronic partition function. Relations of partition function with thermodynamic functions such as internal energy, heat capacity, Entropy & probability, heat content, work function 'A', Gibb's free energy, heat content and third law of thermodynamics and equilibrium constant from partition functions.

**Module III**

**Quantum Statistics** (08 Lectures)

Quantum Statistics- Bose- Einstein & Fermi Dirac statistics and its application, Theories of specific heat of solids classical and Einstein treatment.

**Module IV**

**Surfactants** (10 Lectures)

Introduction: Characteristic features of surfactants and amphiphiles. Various types of amphiphiles. Self-assembly and the critical packing parameter. Factors affecting self-aggregation.

**Module V**

**Experimental Methods for Detection of Self-aggregation** (10 Lectures)

Experimental methods for detection of self-aggregation. Thermodynamic parameters of amphiphilic aggregation. Vesicles, Types of vesicles, Gel-to-liquid crystalline phase transition. Differential Scanning Calorimetry studies. Lichtenberg three stage model.

**Texts Books/Reference Books**

1. Surfactants and Interfacial Phenomena – Milton J. Rosen. John Wiley & Sons, Inc
2. Surfactant Aggregation – J. H. Client. Springer
3. Thermodynamics-A core course – Srivastava, Saha & Jain.
4. Statistical Thermodynamics – M. C. Gupta
5. Fundamentals of classical and Statistical Thermodynamics - B. N. Roy
6. Classical and Statistical Thermodynamics - A. H. Carter

**M.Sc. Chemistry - Semester I (M.Sc. 1-year Program)**  
**Inorganic Chemistry Lab**  
**Subject Code: CH601B4**

**(Credits: Lab-03)**

**Course Objectives**

To gain experience in synthetic techniques and interpretation of the spectra based on concepts learned in theory

**Course/Learning Outcome:**

1. Enable to synthesize different first row transition metal complexes, their purification and crystallization.
2. Enable to determine percentage of yield of the products and to characterize physical properties.
3. Enable to carry out UV-vis spectroscopic studies of the prepared complexes.
4. Enable to carry out FTIR spectroscopic studies of the prepared complexes.
5. Enable to analyse UV-vis and FTIR spectral data (Molar extinction coefficient, identification of d-d transition and charge transfer).

**List of Experiments**

1. Synthesis of first row transition metal complexes and their purification (minimum of 10 complexes).
2. UV-vis spectroscopic studies of the prepared complexes:
  - a) Role of metal ions
  - b) Influence of ligands
  - c) Total interpretation of spectra and correlation with CFT

**Textbooks/Reference Books**

1. Co-ordination Chemistry Reviews
2. Journal of Chemical Education
3. Inorganic Chemistry, Principles of Structure and Reactivity – James E. Huheey, Ellen A. Keiter, Richard L. Keiter

**M.Sc. Chemistry - Semester I (M.Sc. 1-year Program)**  
**Organic Chemistry Lab**  
**Subject Code: CH602B4**

**(Credits: Lab-03)**

**Course Objectives**

This course will help provide hand on experiences of various techniques adopted in organic synthesis. Students will be able to handle various routine techniques used during organic synthesis in laboratory.

**Course/Learning Outcome**

CO1: Learn and apply techniques used purification of organic solvent.

CO2: Apply difference chromatographic techniques used in purification of organic molecules.

CO3: Apply crystallization techniques for purification of organic molecule.

CO4: Explain and estimate the concentration of organic molecule through redox titration.

CO5: Apply various green synthesis techniques for preparation of organic molecule/derivatives.

**List of Experiments**

1. Purification of organic molecules/solvents through normal distillation, distillation under reduced pressure.
2. Hand on experience on thin layer chromatography (TLC) / PTLC, crystallization and Column chromatography for separation/purification of organic molecule.
2. Estimation of Glucose and phenol or acetone through redox reaction.
3. Some Green Organic synthesis
  - (a) Bromination
  - (b) Acetylation
  - (c) Nitration
  - (d) Some name reactions
4. Organic synthesis in solid support. (with or without microwave irradiation)

**Textbooks/Reference Books**

1. Vogel's textbook of practical organic chemistry - Furniss Hannaford Smith, Tatchell
2. Monograph on Green Chemistry – Laboratory Experiment - Green Chemistry task force committee, DS

**M.Sc. Chemistry - Semester I (M.Sc. 1-year Program)**  
**Project Based Learning**  
**Subject Code: CH601B5**

**(Credits: Project-01)**

**M.Sc. Chemistry - Semester II (M.Sc. 1-year Program)**  
**Bio-inorganic Chemistry**  
**Subject Code: CH604B1**

**(Credit: Theory-03)**

**Course Objective**

The students will acquire in-depth knowledge of role of transition metal ions and its complexes in different biological processes and their chemistry in treatment of different diseases.

**Course/Learning Outcome**

CO1: Understanding of basic reactions in the biological systems and storage & transport of metabolic energy.

CO2: Ability to understand ion transport across the biological membrane. To know the working of sodium ion pump.

CO3: In-depth knowledge of biological redox reactions, their importance and dioxygen in biological systems.

CO4: In-depth Knowledge of metalloproteins in biological system and their active site structures.

CO5: Knowledge of metalloenzymes and their applications in biological systems.

**Module I**

**Basic Biological Inorganic Reaction** (08 Lectures)

a) Basic reactions in the biological system and the roles of metal ions. Metal complexes in medicine- cisplatin, auranofin.

b) Metal – nucleic acid interactions - Metal ion interaction with Nucleosides & Nucleotides, Metal ion interaction with DNA, Metal ion interaction with RNA.

c) ATP =ADP Interconversion, Creatine- Phosphocreatine interconversion, phosphate transfer and its activation by metal ions.

**Module II**

**Transport Across Biological Membrane** (08 Lectures)

Transport Across Biological membrane – Ionophores as metal ion carriers- cyclic natural ionophores, open chain carboxylic acid ionophores & other ionophores. Active transport across the membrane, Na<sup>+</sup>/K<sup>+</sup> transporting AT Pase, Na<sup>+</sup> ion pump.

**Module III**

**Biological Redox Reaction** (08 Lectures)

Biological Redox Reaction- Electron transport proteins – Ferredoxins, Cytochromes. Energetics of electron transport in the respiratory chain, Photosynthesis.

Dioxygen in Biological system- Reactions of molecular oxygen, Activation of Dioxygen Molecule in Transition metal Dioxygen complexes.

**Module IV**

**Metalloproteins** (08 Lectures)

Oxygen carrying proteins- Haemoglobin & Myoglobin, Hemerythrin, Hemocyanin, cooperatively in haemoglobin, Bohr effect, Blood Substitute.

Model system- Synthetic oxygen carriers-

(i) Porphyrin Derivatives,

(ii) Cobalt (II) Dioxygen complexes

(iii) Iridium (II) Dioxygen complexes (Vaska's complexes)

(iv) Platinum group metal dioxygen complexes.

## Module V

### **Metalloenzymes**

(08 Lectures)

Redox enzymes- Molybdenum containing enzymes, Iron containing enzymes, Copper containing enzymes, Zinc containing enzymes.

Hydrolytic Enzyme-Carboxy peptidase, carbonic anhydrase

Vitamins & co-enzymes

### **Textbooks/Reference Books**

1. Biochemistry – L. Stryer
2. Principles of Bioinorganic chemistry – S. J. Lippard and J. M. Berg
3. Inorganic Biochemistry – G. L. Eichhorn
4. Elements of Bioinorganic Chemistry – G. N. Mukharjee, A. Das
5. Bioorganic, Bioinorganic and Supramolecular Chemistry – P. S. Kalsi, J. P. Kalsi

**M.Sc. Chemistry - Semester II (M.Sc. 1-year Program)**  
**Solid State Chemistry and Interface Science**  
**Subject Code: CH605B1**

**(Credit: Theory-03)**

**Course Objective**

The course introduces the concept of molecular arrangements within crystalline solids followed by the aggregation of specific molecules into colloids and its applications.

**Course/Learning Outcome**

CO1: Able to understand basic concept of crystal structure, its defect and its application to explain electrical properties of the solid material.

CO2: Able to describe the fundamental concept of Band Theory.

CO3: Understand surface chemistry of adsorption.

CO4: Ability to understand the basics of colloids and their applications.

CO5: Understand the various processes of Photochemistry.

**Module I**

**Solid State Chemistry** (08 Lectures)

Unit cell, Miller indices, Bravais lattice, Bragg's equation, crystal structure analysis, Structure of NaCl, KCl, and Zinc Blende, Types of defects in solids and its influence on electrical properties of solids.

**Module II**

**Band Theory** (08 Lectures)

Band theory and its application, Insulators & semiconductors and its types & preparation, superconductor and its application, Macromolecules: concept molecular mass, its determination.

**Module III**

**Surface chemistry** (08 Lectures)

Adsorption of gases on solids, Freundlich's adsorption isotherm, Langmuir adsorption isotherm, Gibb's adsorption equations, BET Application of Adsorption.

**Module IV**

**Colloids** (08 Lectures)

Association colloids, Preparation of colloidal sol and application of colloidal Science application, Emulsion and micro emulsion formation and thermodynamics application (detergency), Solubilization of surfactant solution Donnan Membrane equilibrium.

**Module V**

**Photochemistry** (08 Lectures)

Einstein law of Photochemical equivalence, quantum yield, primary and secondary processes, Photoelectric effect, Latent Image, Elementary idea of laser and its application.

**Texts Books/Reference Books**

1. Physical Chemistry of Surface – A. W. Adamson & A. Gast
2. Solid State chemistry and Its Applications - Anthony R. West
3. Basic Solid State Chemistry – A. R. West
4. Solid State Chemistry – Kettal
5. Applied colloid and surface chemistry – R. Pashley
6. Colloids and Interface with Surfactants and Polymer – James W Goodwin

**M.Sc. Chemistry - Semester II (M.Sc. 1-year Program)**  
**Group Theory – A Chemist Approach**  
**Subject Code: CH606B1**

**(Credit: Theory-03)**

**Course Objective**

To provide basic understanding of group theory and its application in chemistry. The course will help students to clear the concept of spectroscopy.

**Course/Learning Outcome**

CO1: Ability to identify the symmetry elements and symmetry operation in molecules.

CO2: Ability to identify point group, group multiplication table, subgroups and various groups.

CO3: Ability to make transformation matrix for various symmetry elements.

CO4: Ability to make the character representation of a point group on different basis sets.

CO5: Able to construct character table and apply them to find various properties of molecules.

**Module I**

**Symmetry Elements and Symmetry Operations** (12 Lectures)

Introduction, importance of symmetry, geometry of molecule through VSEPR theory, different symmetry elements, symmetry operation of each symmetry element, horizontal plane, vertical plane, dihedral plane, associated operation of  $S_n$  axis, finding out symmetry elements present in  $AB_2$  (linear and bent),  $AB_3$  (Planar and pyramidal),  $AB_4$  (tetrahedral and planar),  $AB_5$  (planar, trigonal bipyramidal, square pyramidal),  $AB_6$  (planar, octahedral), spiro, cycloalkane [especially cyclohexane (chair, boat)], conformations of ethane (staggered, eclipsed), alkene, alkyne, ferrocene etc, product of symmetry operations, commutative symmetry operation.

**Module II**

**Symmetry Elements and Point Groups** (10 Lectures)

Mathematical rules for the formation of a group, flow chart for determination of point group, symmetry elements present in a point groups, variation of symmetry elements and point group by substitution, order of a group, group multiplication table for a  $C_s$ ,  $C_i$ ,  $C_n$ ,  $C_{nv}$ ,  $C_{nh}$  etc, conjugate elements and classes of different point groups, subgroups of a point group, Isomorphic group, Abelian group, Symmetry number, application of point group on optical activity and dipole moment.

**Module III**

**Matrix Representation of Symmetry Operations** (06 Lectures)

Definition, order, matrix multiplication and addition, transpose of a matrix, inverse of a matrix, Solutions of linear equations by matrix method, transformation matrices for i) identity ii) plane of symmetry iii) centre of symmetry iv) axis of symmetry v) improper axis of symmetry, transformation matrix for  $S_n$  axis.

#### **Module IV**

##### **Representation of Point Groups**

(06 Lectures)

Characteristic of matrix representation, character representation of a point group, method for deriving matrix representations on different basis set, method to directly arrive character representation, classification of representations.

#### **Module V**

##### **Character Table**

(10 Lectures)

The great orthogonality theorem, Application of the orthogonality theorem, construction of character tables, Character table of various point group, Mullikan symbols for IR's, Determination of symmetry species for translations and rotations. IR active and Raman active vibrations.

##### **Texts Books/Reference Books**

1. Chemical Applications of Group Theory – F. A. Cotton
2. Molecular Spectroscopy – D. J. Willock
3. Symmetry and Spectroscopy of Molecules – K. V. Reddy
4. A Simple Approach to Group Theory in Chemistry – S. Swarnalakshmi, T. Saroja, R M Ezhilarasi

**M.Sc. Chemistry - Semester II (M.Sc. 1-year Program)**  
**Quantum Chemistry-II**  
**Subject Code: CH607B1**

**(Credit: Theory-03)**

**Course Objective**

The course aims to introduce students to an advanced state of quantum chemistry where the students will apply the basic principles and model systems of quantum mechanics to real systems with the help of approximation methods

**Course/Learning Outcome:** On successful completion of this course students would be able to  
CO1: Apply Variation method to solve the wave functions of common model systems in quantum chemistry.

CO2: Apply perturbation theory to solve quantum mechanical problems.

CO3: Elucidate the wave functions of He and other multi-electronic systems using approximation techniques.

CO4: Correlate the Born Oppenheimer approximation and MOT with the PE curve of molecules.

CO5: Explain chemical bonding using VB and HMO theories.

**Module I**

**Approximation Methods** (08 Lectures)

Variation method, Linear and nonlinear variation functions and its application in particle in a box, simple harmonic oscillator and hydrogen atom systems.

**Module II**

**Perturbation Method** (08 Lectures)

First and second order corrections and its application in particle in a box, simple harmonic oscillator and hydrogen atom systems.

**Module III**

**Helium Atom and Other Multielectronic Systems** (10 Lectures)

Application to two electron system.: electron spin, spin orbital, Pauli exclusion rule, columbic and exchange energies. Excited state of He atom, symmetric and antisymmetric wave functions.

Multielectron atoms, determinantal form of the wave function, self-consistent field approximation, Hartree-Fock Self Consistent field theory, Slater type orbitals.

**Module IV**

**Molecular Systems** (08 Lectures)

Separation of electronic and nuclear motions treatment of homonuclear and heteronuclear diatomic molecules- the Born Oppenheimer approximation, MO theory, LCAO-MO approximation, MO's of  $H_2^+$  and  $H_2$  molecule.

## Module V

### Valence Bond Theory and Semi Empirical Methods

(10 Lectures)

Valence bond theory, Heitler-London theory, electron density distributions, the Ab-initio calculations semiempirical methods. Huckel theory for linear and cyclic conjugated systems; Applications to simple  $\pi$  systems: Ethylene, vinyl, cyclopropenyl.

### Text Books/Reference Books

1. Quantum Chemistry – Levine
2. Quantum Chemistry – R K Prasad
3. Molecular Quantum Mechanics – P. W. Atkins
4. Quantum Chemistry – Pauling & Wilson
5. Quantum Chemistry – F. L. Pilar
6. Quantum Chemistry – McQuarrie
7. Quantum Chemistry – Eyring, Walter and Kimball

**M.Sc. Chemistry - Semester II (M.Sc. 1-year Program)**  
**Chemistry of Nanomaterials**  
**Subject Code: CH604B3**

**(Credit: Theory-04)**

**Course Objective**

The course introduces the concept of nano science, specifically nano material chemistry and its applications.

**Course/Learning Outcome**

CO1: Explain and identify basic aspects of nanomaterials.

CO2: Ability to generate new methods for synthesis of nanomaterials.

CO3: Demonstrate and identify porous and carbon materials.

CO4: Demonstrate and identify various experimental techniques and characterizations of nanomaterials.

CO5: Apply nanomaterials in various fields of chemistry.

**Module - I**

**Basic Aspects at Nanoscale Materials** (10 Lectures)

Surface plasmon effect, semiconductor nanoparticles, quantum confinement, magic number in clusters, physical chemistry of solid surfaces and at the nanoscale, surface (electrostatic and steric stabilization), bottom-up synthesis approach, nucleation theory, growth mechanisms and its control, Ostwald ripening, Fundamentals of film growth, nucleation process in film formation.

**Module - II**

**Nanomaterial Synthesis** (10 Lectures)

Chemical routes, electrochemical methods and vapor growth. thin films methods, chemical vapor deposition, physical vapor deposition (sputtering, laser ablation) and Langmuir-Blodgett growth. mechanical methods: ball milling and mechanical attrition. sol-gel methods, bioinspired synthesis.

**Module - III**

**Porous and Carbon Materials** (10 Lectures)

Micro and mesoporous materials: zeolites, porous silicon synthesis, formation mechanism, different applications Special nanomaterials: graphene, carbon nanotubes, fullerenes, nanowires.

**Module - IV**

**Overview of Different Characterization Techniques** (10 Lectures)

Overview of different experimental techniques for structural characterization of nanomaterials, Detail of the characterization techniques: X-ray diffractometry (XRD), Scherrer equation, crystal size measurement, transmission electron microscopy (TEM), bright-field and dark field imaging in TEM, selected area electron diffraction, scanning electron microscopy (SEM), BET surface area measurement, scanning tunneling microscopy (STM), atomic force microscopy (AFM).

## **Module - V**

### **Different Applications of Nanomaterials**

(08 Lectures)

Different applications of nanomaterials like in catalysis, environmental, biomedical, solar cells, electronic circuits, light emitting devices, data storage, biological tags, cancer treatments, drug delivery.

### **Texts Books/Reference Books**

1. Inorganic Materials Synthesis and fabrication – John N. Lalena. John Wiley and Sons.
2. Nanochemistry: A chemical approach to nanomaterials – Geoffrey A. Ozin and Andre C. Arsenault. RSC Publishing.

**M.Sc. Chemistry - Semester II (M.Sc. 1-year Program)**  
**Supramolecular Chemistry**  
**Subject Code: CH605B3**

**(Credit: Theory-04)**

**Course Objective**

Introduction to concepts of Supramolecular chemistry, various routes of synthesis, its uses and future possible application

**Course/Learning Outcome**

CO1: Understanding Host-Guest Chemistry, receptors & Macrocyclic effects.

CO2: Understanding of various intermolecular forces and its application in construction of supramolecules.

CO3: Understanding chemistry of formation of various supramolecular systems and their application.

CO4: Knowledge of self-assembly process in construction of supramolecules.

CO5: Understanding the role of coordination chemistry in construction of functional supramolecular materials.

**Module I**

**Introduction** (10 Lectures)

From molecular to supramolecular Chemistry, Factors leading to strong binding, H-bonding and stacking interaction, Host-Guest Chemistry, Development, Classification of Supramolecular Host-Guest Compounds, Receptors, Coordination and the Lock and Key analogy, Chelate and Macrocyclic effects.

**Module II**

**Nature of Supramolecular Interactions** (10 Lectures)

Ion-Ion, Ion-Dipole, Dipole-Dipole, Hydrogen Bonding, Cation- $\pi$  Interaction,  $\pi$ - $\pi$  Interaction, Hydrophobic effect, Van der Waals Bonding Interaction, Cooperativity, Allosteric Systems.

**Module III**

**Supramolecular Systems** (10 Lectures)

Crown ethers, Podands, Cryptands, Spherands, Lariat ethers, Bibrachial Lariat ethers. Introduction, Synthesis, Nomenclature, Solution behaviour and application in specific recognition process.

**Module IV**

**Supramolecular Assembly of Complex Architectures** (09 Lectures)

Novel Supramolecular Architectures – Catenanes, Rotaxanes, Knots, Cyclodextrins, Cyclophanes, Siderophores. Porphyrins and its Derivatives for construction of Supramolecular Assemblies.

**Module V**

**Coordination Chemistry Based Approach for Functional Supramolecular Materials**

(09 Lectures)

Weal Link Approach, General strategy of WLA, components of WLA, Hemilabile ligands, Ancillary ligands, Functional supramolecular systems, host-guest as molecular sensors, catalytic systems, multivalency and cooperativity, Self-Assembled Molecular Flasks.

### **Texts Books/Reference Books**

1. Supramolecular Chemistry by J. W. Steed & J. L. Atwood, published – Wiley
2. Supramolecular Chemistry by J.M. Lehn, published – Wiley – VCH
3. Review Articles
  - a) Development of a Coordination Chemistry- Based Approach for Functional Supramolecular Structures–Account of Chemical Research, Vol.38, No.11, 825-837, 2005
  - b) Multivalency and Cooperativity in Supramolecular Chemistry– Account of Chemical Research Vol.38, No.9.,723-732,2005
  - c) Functional Molecular Flasks: New Properties and Reactions within Discrete, Self-Assembled Hosts– Angew Chem. Int. Ed., 48, 3418-3438, 2009

**M.Sc. Chemistry - Semester II (M.Sc. 1-year Program)**  
**Medicinal Chemistry**  
**Subject Code: CH606B3**

**(Credit: Theory-04)**

**Course Objective**

This paper will introduce drug design and their synthetic approach. Moreover, Cell structure, Protein structure, Drug action, RNA, DNA, Prodrugs etc will also be discussed. This will also give the idea of various syntheses and applications of Antipyretic Analgesics, Antibacterial agents, Antibiotics, Anti-ulcer agents, Local - Anaesthetics, Anti-cancer agents and Antimalarial.

**Course/Learning Outcome**

CO1: In-depth understanding of mode of action of drugs.

CO2: Synthesis and ability to establish structure-activity relationships of various classes of drug.

CO3: Understanding the role and function of Antihistamines.

CO4: Expertise in synthesis and classifications of various classes of local Anaesthetics.

CO5: In-depth understanding of various classes of Antimalarial drugs.

**Module I**

**Introduction**

(12 Lectures)

Cell structure and Protein structure. Pharmacodynamic, pharmacokinetic (drug adsorption, distribution, metabolism, and elimination) and toxicological aspects of stereoisomers (Geometrical, optical, and conformational). Drug action at Proteins, Drug action at enzymes, competitive and non-competitive inhibitors, Drug action at receptors, the drug receptor, the drug receptor interaction. Stages of drug discovery, lead discovery, identification, validation, and diversity of drug targets. Structure-activity relationships: Strategies in drug design. QSAR and combinatorial synthesis. Optimization of drug-target interactions and access to drug targets.

**Antipyretic Analgesics**

(04 Lectures)

Aniline and p-Aminophenol – Paracetamol, Phenacetin, Acetanilide. Salicylic acid analogues – Aspirin, Salol. N-Aryl anthranilic acid -- Mefenamic acid, Meclofenamate sodium.

**Module II**

**Antibacterial Agents**

(06 Lectures)

The bacterial cell, Mechanisms of antibacterial action. Sulphonamides and Sulphones – Development of sulphonamides as drug – Prontosil, sulphapyridine. Sulphonamides for general infection – Sulphanilamide, Sulphapyridine, Sulfathiazole, Sulfadiazine. Sulphonamides for Urinary infections – Sulfacetamide. Sulphonamides for Intestinal Infections – Phthalyl sulfathiazole, Succinyl sulphathiazole. Sulphonamides for Local Infection – Sulfacetamide, Mafenide. Sulphones --- Dapsone.

**Antibiotics**

(04 Lectures)

The Penicillin, General introduction to  $\beta$ - lactam antibiotics – Cephalosporins, Chloramphenicol, Tetracyclines – structure action relativity.

**Module III**

**Local Anesthetics**

(07 Lectures)

Esters – Ethyl p-aminobenzoate, Butamben, Procaine hydrochloride, Tetracaine hydrochloride. Piperidine or Tropone derivatives – Eucaine, Benzamine hydrochloride. Amides – Lignocaine, Prilocaine, Mepivacaine hydrochloride, Pyrrocaine hydrochloride. Miscellaneous Type – Phenacaine hydrochloride, Eugenol, Mode of action of some selected local anaesthetics.

## **Module IV**

### **Antihistamines**

(07 Lectures)

Histamine H1-receptor Antagonists – Aminoalkyl ethers, Ethylenediamines, Thiophene derivatives, Cyclic basic chain analogues. Histamine H2 Receptor blockers - Peptic ulcers, Histamine Cimetidine – a rational approach to drug design, Cimetidine, ranitidine, famotidine and nizatidine.

## **Module V**

### **Antimalarials**

(08 Lectures)

Prevention of malaria, malarial parasites, Plasmodia, and their life cycle. 4-aminoquinoline – Structure activity relationship, chloroquine, Sontoquine. 8-amonoquinolines – structure activity relationship, pamaquine, primaquine – synthesis, absorption, distribution and excretion, toxicity, uses, routes of administration and dosage. 9-Aminoacridines – Mepacrine hydrochloride, Pyrimidines – Pyrimethamine.

### **Texts Books/Reference Books**

1. An Introduction to Medicinal Chemistry – Graham L. Patrick (Oxford)
2. Medicinal Chemistry – Ashutosh Kar

**M.Sc. Chemistry - Semester II (M.Sc. 1-year Program)**  
**Research Project Work**  
**Subject Code: CH602B6**

**(Credit: Research Project Work-04)**

**Course Objective**

Each Faculty member will provide a research topic to the student(s) from current research area at beginning of 1<sup>st</sup> semester. Each research project topic is different from other. Research Students will perform their research in chemistry lab from 1<sup>st</sup> semester. Students will get an exposure about the research in chemistry.

# **Syllabus for M.Sc. 2-years Program**

**M.Sc. Chemistry - Semester I (M.Sc. 2-years Program)**  
**Principles of Inorganic Chemistry**  
**Sub Code: CH501B1**

**(Credit: Theory-04)**  
**Course Objective**

The course aims to strengthen the fundamentals of inorganic chemistry covering main group elements and inner transition elements.

**Course/Learning Outcome**

CO1: Identify and explain periodic properties of elements, structure and bonding in molecules, to assign structure and deduce properties of a given molecules.

CO2: Explain magnetic properties of molecules, and their application in deducing properties of a molecule.

CO3: Demonstrate synthesis, properties bonding of p-block elements and their compounds and applications.

CO4: Enable student to understand the synthesis, properties bonding of Boranes, Carboranes, Metallo-carboranes, Borazines, Phosphazenes, Sulfur-Nitrogen compounds, silicates, silicones. Iso- and Hetero-poly anions. Understand the concept of allotropy and its significance.

CO5: Enable student to understand Metal-Metal bonds, industrial importance of the compounds of main group elements. Brief review of inorganic chains, rings and cages, organometallic compounds of non-transition elements.

**Module I**

**Structure and Bonding** (10 Lectures)

Structure and bonding in homo- and heteronuclear molecules: VSEPR Theory, VBT, MOT, Bent's rule, Fajan's rule, physical properties of molecules, (bond energies, force constants, bond lengths bond polarities and electronegativity).

**Module II**

**Magnetic Properties** (08 Lectures)

Introduction of magnetic properties, paramagnetism, ferro and antiferro magnetism, diamagnetism, Pascal constants, Currie equation, determination of magnetic susceptibility. Orbital magnetic moment, spin magnetic moment, spin-orbit coupling, Russell-Saunders, j-j coupling scheme, quenching of orbital angular momentum by ligand fields, the Zeeman effect.

**Module III**

**Main Group Elements and Their Compounds** (12 Lectures)

Synthesis, properties, structure and bonding of nitrogen, phosphorous, sulfur, pseudohalogen, Interhalogen and xenon compounds.

**Module IV**

**Brief Review of Inorganic Chains, Rings and Cages** (10 Lectures)

Boranes, carboranes, metallo-carboranes, the isolobal analogy Borazines, phosphazenes, sulfur-nitrogen compounds, silicates, silicones. iso- and hetero-poly anions, allotropy.

## Module V

### General Periodic Trends

(08 Lectures)

Metals, compounds containing metal-metal bonds, metal clusters metal-metal quadruple and triple bonds, some reactions of compounds involving metal-metal multiple bonds, organometallic compounds of non-transition elements.

### Textbooks/Reference Books

1. Inorganic Chemistry, Principles of Structure and Reactivity - James E. Huheey, Ellen A. Keiter, Richard L. Keiter
2. Advanced Inorganic Chemistry – F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann
3. Inorganic Chemistry - Shriver and Atkins
4. Inorganic Chemistry – G. L. Miessler, P. J. Fischer & D. A. Tarr

**M.Sc. Chemistry – Semester I (M.Sc. 2-years Program)**  
**Principle of Organic Chemistry**  
**Subject Code: CH502B1**

**(Credits: Theory-04)**

**Course Objective:** This course gives the idea of MO's theory, acid-base concept, stereochemistry, Organic reaction intermediate.

**Course Outcome:**

CO1: Apply MOT for predicting reaction mechanisms.

CO2: Identify problems related to stereochemistry.

CO3: Explain and identify the role of carbocation in organic synthesis and nucleophilic substitution reaction.

CO4: Explain and identify the role of carbanion in organic synthesis and nucleophilic substitution reaction.

CO5: Explain and identify the role of neutral intermediate in organic synthesis and nucleophilic substitution reaction.

**Module - I**

**Principle of MO's Theory and its Application to Reactivity** (10 Lectures)  
Introduction, Molecular orbital - homonuclear, heteronuclear (both sigma and pi-bonded molecule), delocalization, tautomerism, aromaticity, anti-aromaticity etc. Huckel molecular orbital theory.

**Module -II**

**Stereochemistry II** (10 Lectures)  
Isomers – Classes of isomers, Isomerism – optical and geometrical Isomerism, Nomenclature of enantiomers – R.S. & E.Z. system. Elements of symmetry, Concept of chirality, Centre of chirality - molecules with C, N, S based chiral centers, molecules with more than one chiral center. Methods of resolution, optical activity in absence of chiral carbon, atropisomerism.  
Conformation analysis of cycloalkanes: Meaning of conformation, Effect of conformation on the stability and reactivity, Stereochemistry of six-membered rings, Mono-substituted and disubstituted cyclohexane, Decalines, Gauche butane interactions in substituted cyclohexanes and decalines.

**Module -III**

**Reactive Intermediates - I** (08 Lectures)  
Carbocation: Structure, and stability of carbocations, Classical and non-classical carbocation, C-C bond formation involving carbocations, Oxymercuration, halolactonisation. Acetal formation, Friedel-crafts reaction, Wagner-Meerwein rearrangement, Hydroperoxide rearrangement.

**Module -IV**

**Reactive Intermediates - II** (08 Lectures)  
Carbanion: Structure and stability, Chemistry of enolates and enamines, Kinetic and thermodynamic enolates, alkylation and acylation of enolates, Nucleophilic additions to carbonyls, Introduction of Favorskii and Neber rearrangement.

## Module -V

### Reactive Intermediates - III

(12 Lectures)

Free radicals: Generation, structure, and stability of radical intermediates and their (a) addition to alkenes, alkynes (inter & intramolecular) for C-C bond formation (b) fragmentation and rearrangements.

Carbenes: Generation, structure and stability, Addition and insertion reactions.

Nitrenes: Generation, structure and stability, Reactions of nitrene and related electron deficient nitrogen intermediates, Hoffmann, Schmidt, Beckmann rearrangement reactions. Curtius rearrangement –mechanism challenges. Effect of structure on reactivity, The Hammett equation and linear free energy relationship (sigma-rho), Taft equation.

### Textbooks/Reference Books

1. Organic Chemistry, vol. I & II (ELBS) - Finar, I. L
2. Advanced Organic Chemistry -J. March, Willey Interscience
3. Organic Chemistry - O. P. Agrawal
4. A Guidebook to Mechanism in Organic Chemistry by Peter Sykes
5. Stereochemistry – Eliel
6. Stereochemistry – D. Nasipuri
7. Organic Chemistry – J. Clayden, N Greeves, S. Warren & P. Wothers

**M.Sc. Chemistry - Semester I (M.Sc. 2-years Program)**  
**Chemical Thermodynamics**  
**Sub Code: CH503B1**

**(Credits: Theory-04)**

**Course Objective**

The study of entropy, free energy and work function relation with the change of various conditions and their mathematical application to understand third law, chemical potential, the phase equilibrium and statistical thermodynamics.

**Course/Learning Outcome:**

CO1: Analyse fundamental concepts of solution thermodynamics involving ideal and non-ideal systems.

CO2: Explain solution thermodynamic concepts and phase equilibria in two-component and multi-component systems.

CO3: Explain Entropy of mixing and Work function.

CO4: Explain colligative properties and Raoult's law.

CO5: Explain Gibbs Duhem equation.

**Module I**

**Concept of Entropy**

(10 Lectures)

Entropy, Nature of  $dq$  and  $dq/T$ , Physical Significance of Entropy, Entropy of a Perfect Gas, Change of entropy with temperature and pressure, Entropy of mixing, Work function or Helmholtz free energy  $A$  and Gibbs free energy or Gibbs potential & their variation with the parameters of the system, Maxwell thermodynamic relation and its applications.

**Module II**

**Colligative Properties**

(10 Lectures)

Clapeyron Clausius equation with derivation & application to various phase equilibrium, & Colligative properties - elevation of boiling point and depression of freezing points, Van't Hoff law of mass action & reaction isotherm, isochore, Raoult's law and its application.

**Module III**

**Gibb's Helmholtz Equations**

(08 Lectures)

Limitation of Gibb's Helmholtz concepts, Nernst heat theorem, its proof and application, Third law of thermodynamics, its application and exception of third law.

**Module IV**

**Gibbs Duhem Equation**

(10 Lectures)

Gibbs Duhem equation for open system, Thermodynamic criteria for equilibrium in open system, Concept of Fugacity & Activity, their significance, variation of Fugacity & Activity of a gas with pressure and temperature.

## Module V

### Reduced Phase Rule

(10 Lectures)

Reduced Phase rule, Eutectic systems as lead silver system, potassium iodide-water system, Binary alloys system with congruent and incongruent melting points.

### Textbook/Reference Books

1. Advance Physical Chemistry – D. N. Bajpai
2. Physical Chemistry – Silbey & Alberty
3. Physical Chemistry – Atkins
4. Physical Chemistry of Molecular Approach – Mc. Quarrie & Simon
5. Fundamentals of classical and Statistical Thermodynamics - B. N. Roy
6. Classical and Statistical Thermodynamics - A. H. Carter

**M.Sc. Chemistry - Semester I (M.Sc. 2-years Program)**  
**Analytical Chemistry**  
**Subject Code: CH504B1**

**(Credits: Theory-04)**

**Course Objectives**

The course aims to introduce students to the fundamental principles of Analytical Chemistry. The course introduces the concept of errors and correct techniques for sampling and then delves into the various aspects of analytical chemistry viz, chemometrics, separation techniques followed by analytical techniques including instrumental methods of analysis

**Course/Learning Outcome:** On successful completion of this course students would be able to

CO1: Understand the scope of analytical chemistry and principles of chemometrics.

CO2: Discuss structure, factors and application of macrocyclic compounds and resins in separation.

CO3: Apply chromatographic techniques for separation of compounds.

CO4: Use solubility principles for quantitative precipitation of compounds.

CO5: Derive titration curves from basic principles of titrimetric analysis.

**Module I**

**Introduction to Analytical Chemistry** (10 Lectures)

Scope, methods of quantitative analysis, selection of method of analysis, steps in quantitative analysis and role of instrumentation in analytical chemistry.

Errors, classification of errors, determining and improving of accuracy in analysis, significant figures, distribution of random errors, Confidence interval, Comparison of results, student t-test, comparing the means of two samples, paired t test, F test, Q test, rejection of results, Correlation and Regression.

**Module II**

**Separation Techniques** (10 Lectures)

Crown ethers, cryptands and calixarenes in solvent extraction: classification, structure factors influencing solvent extraction and applications.

Ion exchange chromatography: characteristics of ion exchange resins, synthesis of ion exchange resin, classification of ion exchange resins, mechanism of ion exchange and equilibria, factors affecting ion exchange, Applications of ion exchange in deionization of water, metal separation.

**Module III**

**Chromatography** (10 Lectures)

High performance liquid chromatography: Plate theory for chromatography, Van-Deemter Equation, Instrumentation, working and applications of HPLC. Supercritical fluid chromatography, Instrumentation, working, applications and comparison with HPLC and GC.

Gas chromatography – Principles, instrumentation, working and applications.

**Module IV**

**Gravimetric and Thermal Analysis** (10 Lectures)

Solubility, solubility product, fractional precipitation, quantitative effects of common ion. degree of dissociation of weak acids and bases. Gravimetric analysis, precipitation methods, purity of precipitate (co precipitation), optimum condition for precipitation, precipitation from homogeneous

solution, washing and ignition of the precipitate, role of organic precipitate, criteria for choice of organic reagent, important organic precipitants. Numerical problems based on gravimetric analysis of mixtures.

Thermal Methods of Analysis: Thermogravimetric Analysis, DTA, DSC Instrumentation, Principles and their applications.

### **Module V**

#### **Titrimetric Analysis**

(08 Lectures)

Classification, basic principles of each class of titrations, theory of indicators, Titration curves for neutralization and redox titrations, Selectivity, Masking and demasking in complexometric titrations.

#### **Textbooks/Reference Books**

1. Analytical Chemistry – S. M. Khopkar
2. Vogel's Quantitative Chemical Analysis – J Mendham, R C Denney, J D Barnes, M J K Thomas
3. Instrumental methods of analysis – Willard, Merit & Dean
4. Analytical Chemistry – Gray D. Christian

**M.Sc. Chemistry - Semester I (M.Sc. 2-years Program)**  
**Physical Chemistry Lab**  
**Subject Code: CH501B4**

**(Credit – Lab 03)**

**Course Objectives**

The course aims to enable the students to understand the practical aspects of Physical Chemistry.

**Course/Learning Outcome**

CO1: Ability to apply basic techniques of solution preparation and determine the aggregation process through viscometry and conductometric methods.

CO2: Understand the experimental procedure to determine the kinetic parameters of selected reactions.

CO3: Ability to apply the knowledge of conductometric and potentiometric titration for determination of solubility of sparingly soluble salts.

CO4: Ability to determine the composition and complex formation through spectroscopic analysis.

CO5: Ability to execute electrochemical oxidation and reduction of  $K_3[Fe(CN)_6]/K_4[Fe(CN)_6]$  system by cyclic voltametric technique.

**List of Experiments**

1. To study the kinetics of iodination of acetone spectrophotometrically
2. To study the adsorption of acetic acid by activated charcoal from an aqueous solution
3. To determine the CMC of surfactant by surface tension method
4. To determine the CMC of surfactant by conductivity method
5. To determine the CMC of surfactant by spectrophotometer method
6. To determine the molecular mass of a polymer by viscosity method
7. To determine the energy of activation of hydrolysis of methyl acetate catalysed by hydrochloric acid
8. To determine the second order rate constant for the hydrolysis of ethyl acetate by sodium hydroxide conductometrically
9. To determine the dissociation constant of an indicator, methyl red by spectrophotometric method
10. Determination of the concentration of sulphuric acid, acetic acid and copper sulphate by conductometric titration
11. To determine the formula of the complex formed between copper (II) ion and ammonia
12. To study the redox behaviour of  $K_3[Fe(CN)_6]/K_4[Fe(CN)_6]$  by cyclic voltammetry

**Texts Books/Reference Books**

1. Experimental Physical Chemistry – V. D. Athawale & Parul Mathur
2. Practical in Physical Chemistry – A Modern Approach - P. S. Sindhu
3. Experimental Physical Chemistry – Shoemaker & Nibler
4. Experimental Physical Chemistry – Farrington Daniels
5. Findlay's Practical Physical Chemistry - B. P. Levitt

**M.Sc. Chemistry - Semester I (M.Sc. 2-years Program)**  
**Analytical Chemistry Lab**  
**Sub Code: CH502B4**

**(Credits: Lab-03)**

**Course Objectives**

The course aims to enable the students to apply the principles of analytical chemistry to the analysis of unknown chemical samples. This course is meant to complement the theoretical course.

**Course/Learning Outcome**

CO1: Independently perform separation of components.

CO2: Perform accurately volumetric and gravimetric analysis.

CO3: Ability to analyse results.

CO4: Ability to perform quantitative estimation of alkali ions.

CO5: Interpret UV-Vis and FTIR Spectra.

**List of Experiment of Analytical Chemistry Laboratory**

1. Volumetric Analysis
  - i) Acid - Base – Neutralization
  - ii) Redox Titration (Including Iodometric Titration)
  - iii) Precipitation Titration
  - iv) Complexometric Titration
2. Gravimetric Analysis: At least one experiment involving each of the following:
  - i) High temperature ignition compounds
  - ii) Use of organic precipitants
  - iii) Precipitation from Homogenous solutions
3. Solvent Extraction Experiments (Separation Volumetric Analysis may be combined)
4. Flame Photometry
  - i) Estimation of  $\text{Na}^+$
  - ii) Estimation of  $\text{K}^+$
  - iii) Estimation of  $\text{Na}^+$  and  $\text{K}^+$  in a mixture
5. Spectrophotometric Analysis: Iron and Copper
6. Demonstration of the following experiments:
  - i) TGA & DSC
  - ii) Cyclic Voltammetry
  - iii) Florescence Spectroscopy

**Textbooks/Reference Books**

1. Analytical Chemistry – S. M. Khopkar
2. Vogel's Quantitative Chemical Analysis – J Mendham, R C Denney, J D Barnes, M J K Thomas
3. Instrumental methods of analysis – Willard, Merit & Dean
4. Analytical Chemistry- Gray D. Christian

**M.Sc. Chemistry - Semester II (M.Sc. 2-years Program)**  
**Modern Spectroscopic Techniques**  
**Subject Code: CH505B1**

**(Credits: Theory-04)**

**Course Objective**

Introduction to various techniques of spectroscopy used in chemistry. Detailed interpretation of spectra to identify unknown compounds. Introduction to advanced techniques for interpretation of complex spectra.

**Course/Learning Outcome**

CO1: Explain fundamentals of spectroscopy and solve numerical problems (determination of spectroscopic quantities, molar absorption coefficient).

CO2: Explain fundamentals of rotational spectroscopy, interpret spectra and solve numerical problems (determination of rotational constants, bond length).

CO3: Demonstrate fundamentals of vibrational spectroscopy, interpret spectra and solve numerical problems. (determination of force constant/bond energy). Explain fundamentals of Raman spectroscopy and structure determination.

CO4: Elucidate fundamentals of electronic spectroscopy of atoms and molecules, interpret spectra and solve numerical problems.

CO5: Explain fundamentals of NMR and EPR spectroscopy, interpret spectra and solve numerical problems.

**Module I**

**Introduction to Molecular Spectroscopy** (08 Lectures)

Characterization of electromagnetic radiation, quantization of energy, S/N ratio, width and spectral intensity of spectral transition, F.T. Spectroscopy, stimulated emission. Types of molecular spectroscopy different types of molecular energies, Boltzmann distribution.

**Module II**

**Microwave Spectroscopy** (08 Lectures)

Introduction, rotational energy level, selection rule, simple harmonic oscillator, anharmonic oscillator, bond-distance of a diatomic molecule, relative population and intensity of the absorption peaks, polyatomic molecules, limitations of microwave spectroscopy.

**Module III**

**Infrared and Raman spectroscopy** (12 Lectures)

Introduction, the range of infrared spectroscopy, theory of I.R., SHO, vibrating diatomic molecule as anharmonic oscillator, diatomic molecule as a harmonic oscillator and a rigid rotator, interaction of rotations and vibrations, polyatomic molecules, limitations of I. R. spectroscopy.

Raman Spectroscopy – pure rotational Raman spectra, vibrational Raman spectra, polarization of light and the Raman effect, structure determination from Raman and I. R. spectroscopy, techniques and instrumentation, near IR FT-Raman spectroscopy.

## Module IV

### Electronic Spectroscopy (12 Lectures)

Electronic Spectroscopy of Atoms – Electronic wave functions, energies of atomic orbitals, electronic angular momentum, hydrogen atom spectrum, spectrum of many electron atoms, term symbols, microstate table, photoelectron spectroscopy, Zeeman effect.

Electronic Spectroscopy of Molecules – Born-Oppenheimer Approximation, vibrational-electronic spectra, Franck Condon Principle, dissociation energy and products, fine structure, Fortrat diagram, change of shape on excitation, chemical analysis by electronic spectroscopy.

## Module V

### Spin Resonance Spectroscopy (08 Lectures)

NMR; NMR absorption by nuclei. Theory of NMR spectra, Spin-Spin and Spin-Lattice Relaxation, Multiple Pulse FT, chemical shift, shielding effects, deshielding effects, coupling constant, exchange phenomena, simplification of complex spectra, <sup>13</sup>C NMR, Spectroscopy - double resonance. Application- structure determination, Keto-enol Tautomerism, limitations of NMR spectroscopy. Electron paramagnetic resonance – Theory of EPR spectra. Application- structure determination.

### Texts Books/Reference Books

1. Fundamentals of Molecular Spectroscopy – C. N. Banwell and E. N. McCash
2. Modern Spectroscopy – J. Michael Hollas
3. Symmetry and Spectroscopy – Daniel C. Harris
4. Spectroscopic Methods in Organic Chemistry – H. D. Williams and I. Flemming
5. Organic Spectroscopy – William Kemp
6. Spectroscopy of Organic Compounds – P. S. Kalsi

**M.Sc. Chemistry - Semester II (M.Sc. 2-years Program)**  
**Organic Reactions and Mechanisms**  
**Sub Code: CH506B1**

**(Credits: Theory-04)**

**Course Objective**

This course will give an idea about organic reaction mechanism, substitution, elimination, addition reaction. This will also highlight molecular rearrangement reactions.

**Course/Learning Outcome**

CO1: Assess various aspects of a reaction mechanism to establish it.

CO2: Identify and apply substitution reaction based on substrate nature, used reagents and reaction conditions in organic synthesis.

CO3: Explain and identify the type of rearrangement reactions

CO4: Identify and apply elimination reaction based on substrate nature, used reagents and reaction conditions in organic synthesis.

CO5: Identify and apply addition reaction based on substrate nature, used reagents and reaction conditions in organic synthesis.

**Module I**

**Mechanism and its Investigation** (10 Lectures)

Introduction, Energy profile diagram, Thermodynamics and kinetics requirement for reactions, Thermodynamic vs kinetic control, Hammond's postulate. Methods of determining mechanism - characterization of intermediate, nature of products, solvent effect, isotope effect, kinetic evidence, stereochemical evidence, microscopic reversibility, conclusion.

**Module II**

**Aliphatic & Aromatic Nucleophilic Substitutions** (08 Lectures)

Definition of substitution reaction, types, The SN1, SN2 mechanisms, factors affecting the mechanism, neighbouring group effect, SNi, SN1', SN2/Nucleophilic substitution at an allylic, vinyl carbon, Nucleophilic aromatic substitutions, Benzyne, SNAr mechanism.

**Module III**

**Molecular Rearrangement** (09 Lectures)

Definition, Types of rearrangement reaction, 1,2-Rearrangement – types and examples, Pinacol-pinacolone rearrangement, Dienone-phenol rearrangement, Benzil-benzilic acid rearrangement, Wolff rearrangement, Tiemann rearrangement, The Arndt-Eistert synthesis, The Baeyer-Villiger rearrangement, The Wittig Rearrangement, The Wallach rearrangement.

**Module IV**

**Elimination Reactions** (09 Lectures)

Definition, types and examples, Beta Elimination, Alpha elimination, Cis eliminations, Discussion of E1, E2, E1CB Mechanism and orientation. Orientation of the double bond, Saytzeff and Hofmann

rules. Stereochemistry of E2 reactions. Pyrolytic eliminations, Stereochemistry of syn- elimination, Eliminations Vs substitutions.

Reaction formation of Carbon-carbon and carbon-heteroatom multiple bonds - Shapiro reaction, Peterson reaction, Julia reaction, deoxygenation of *vic*-diol, Ramberg-Bäcklund reaction, Dehalogenation of vicinal dihalides.

## Module V

### Addition Reactions

(12 Lectures)

Definition, Addition to multiple bonds, electrophilic addition mechanism, Markownikoff's rule, Kharasch effect, Nucleophilic mechanism, Addition to diene, Cyclic mechanism (Diels-Alder reaction), Addition to C-C double and C-C triple bond - halogenations, addition of amine, ene reaction, Michael reaction, 1,4-addition, alkylation, acylation, reaction with OsO<sub>4</sub>, and KMnO<sub>4</sub>, Prevost reaction, 1,3-dipolar addition,

Addition to C-O double bond - Formation of acetal and ketal, formation of dithiane, Formation of imine and enamine, Stork enamination reaction, Mannich reaction, Grignard reaction, Claisen condensation, Strecker synthesis, Prins reaction,

Addition to C-N double and C-N triple bond - hydrolysis (acid or base catalysis), addition to amine, Thorpe reaction, Ritter reaction.

### Textbooks/Reference Books

1. Advanced Organic Chemistry – J. March, Wiley Interscience
2. Mechanism and Structure in Organic Chemistry – E. S. Gould (Holt, Rinehart and Winston)
3. A Guidebook to Mechanism in Organic Chemistry – Peter Sykes
4. Organic Chemistry – J. Clayden; N. Greeves; S. Warren; P. Wothers

**M.Sc. Chemistry - Semester II (M.Sc. 2-years Program)**  
**Biochemistry**  
**Subject Code: CH507B1**

**(Credits: Theory-04)**

**Course Objective**

The objective of this paper is to introduce the chemical nature of biomolecules and various types of biochemical reactions involved in chemistry of life. Biochemistry is a well-established exciting discipline, and a very promising research area for M.Sc. Chemistry pass outs.

**Course/Learning Outcomes**

CO1: Apply basic knowledge of biomolecules, biochemical solvents, important functional groups, importance of non-covalent bonds in biochemistry and biochemical thermodynamics.

CO2: Demonstrate fundamental knowledge of four classes of protein structure and their associated functions.

CO3: Demonstrate basic knowledge of different classes of carbohydrate and lipid structures and their associated functions.

CO4: Apply knowledge and understanding of different types of enzymes and enzyme kinetics

CO5: Apply basic understanding of DNA and RNA structure, genetic code, protein synthesis and genetic control.

**Module I**

**Introduction to Biochemistry**

(10 Lectures)

Functional groups of biochemical importance

Water as a biochemical solvent, unique physico-chemical properties of water, importance of hydrogen bond in water and biomolecules, Biochemical evolution of life, how do cells use energy? – connection between metabolic reactions and energy, Spontaneity in biochemical reactions – connections thermodynamics and life, Biochemical aspects of cellular structure, Microscopy in biochemistry – standard light microscope, scanning and transmission electron microscopes – SEM & TEM.

**Module II**

**Protein**

(10 Lectures)

Basic structure of amino acids, stereoisomerism, classification of 20 essential amino acids.

Peptide bond and primary structure of protein, Alpha helix and beta pleated sheet structure of protein (secondary structure), Supramolecular structure of collagen triple helix with functional importance, Tertiary structure of protein with special reference to myoglobin, important non-covalent and hydrophobic interactions in tertiary structures, Application of XRD and NMR techniques to delineate tertiary structures, Quaternary structures of protein with special reference to Haemoglobin.

**Module III**

**Carbohydrate and Lipid**

(08 Lectures)

Carbohydrate – Monosaccharide, disaccharide and polysaccharide.

Lipid metabolism – Fatty acids, fatty acid breakdown, properties and functions of triglycerides, phospholipids and glycolipids.

#### **Module IV**

##### **Enzymes and Enzyme Kinetics** (10 Lectures)

General characteristics and the role of enzymes, holoenzyme, apoenzyme, coenzymes, prosthetic groups. Factors affecting enzyme activity- pH, temperature, enzyme and substrate concentrations, Allosteric enzymes, Cooperativity, concerted and sequential models.

What makes enzymes such effective biological catalysts? How can we describe enzyme kinetics in mathematical terms? How do substrates bind to enzymes? Michaelis-Menten equation for unimolecular reaction.

Reversible and irreversible inhibition; competitive, non-competitive and uncompetitive inhibitions with determination of  $K_M$  and  $V_{max}$ .

#### **Module V**

##### **Nucleic Acids** (10 Lectures)

Basic structure of nucleotides. Formation of dinucleotides and polynucleotides. Structure of DNA. X-ray diffraction double helix model of DNA. Features of DNA molecule. Structure of RNA. DNA replication. DNA replication is semiconservative. About genes. Genetic code. Genetic code is triplet code. Evidence for a triplet code. Breaking the genetic code. Features of genetic code. Transcription. Protein synthesis. Non-coding DNA. Introns and exons. Gene control. Jacob-Monod hypothesis of gene control. Enzyme Induction. Control of metabolic pathways. Modification to the operon hypothesis.

##### **Textbooks/Reference Books**

1. Biochemistry – Lehninger
2. Instant Notes in Biochemistry – B D Hames, N M Hooper & J D Houghton Viva Books Private Limited
3. Biochemistry – Mathews & Holde Pearson Education
4. Biochemistry – Campbell & Farrell Thompson
5. Biological Science by Taylor & Green Cambridge University Press
6. Biochemistry – Rastogi Tata McGrawHill
7. Modern Biotechnology – S B Primrose Blackwell Scientific Publication

**M.Sc. Chemistry - Semester II (M.Sc. 2-years Program)**  
**Quantum Chemistry-I**  
**Subject Code: CH508B1**

**(Credits: Theory-04)**

**Course Objective**

The aim of this course is to make students understand the limitations of classical mechanics and the need of quantum chemistry, familiarize them with postulates of quantum chemistry and apply the same to derive equations for various models and hydrogen atoms. Understand the basis of molecular spectroscopy and its applications.

**Course/Learning Outcome**

CO1: Analyse limitations of classical mechanics and solution in terms of quantum mechanics for atomic/molecular systems.

CO2: Explain and understand of quantum mechanical operators.

CO3: Analyse quantization, probability distribution, uncertainty principle.

CO4: Identify application of quantization to spectroscopy.

CO5: Interpret various types of spectra and know about their application in structure elucidation.

**Module I**

**Beginning of Quantum Mechanics** (10 Lectures)

Black body radiation, Planck's hypothesis of Black Body radiation. Wave-particle duality, light as particles: photoelectric and Compton effects; electrons as waves and the de Broglie hypothesis; Uncertainty relations (with proof). Uncertainty of energy and time.

**Module II**

**Concept of Operators** (10 Lectures)

Elementary concepts of operators, Algebra of Operators, quantum mechanical operators: Commutation of operators, commutator and uncertainty relation, Linear operators, linear and Angular momentum operators, eigenfunctions and eigenvalues; Linear operators; Expectation value; Properties of Hermitian operator. Postulates of quantum mechanics.

**Module III**

**Wave Equation** (10 Lectures)

Theory of wave motion, Classical wave equation, separation of variables, Wave functions and meaning, Acceptable wave functions, Normality and Orthogonality of wave functions, Schrödinger equation and its application to free particle and "particle-in-a-box" (rigorous treatment), quantization of energy levels, zero-point energy Extension to two- and three-dimensional boxes, separation of variables, degeneracy.

## Module IV

### Rigid Rotator

(08 Lectures)

Rigid rotator model of rotation of diatomic molecule. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution.

## Module V

### Vibrational Spectroscopy

(10 Lectures)

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

### Textbooks/Reference Books

1. R. K. Prasad. Quantum Chemistry, New Age International Publishers (Fourth revised Edition).
2. Puri, B. R.; Sharma, L. R.; Pathania, M. S. Principles of Physical Chemistry, Vishal Publishing Co.; 47th Ed. (2017)
3. Kapoor, K. L. A Textbook of Physical Chemistry (Volume 1) McGraw Hill Education; Sixth edition (2019)

**M.Sc. Chemistry - Semester II (M.Sc. 2-years Program)**  
**Dissertation**

**Subject Code: CH505B6**

**(Credits: Dissertation-04)**

**M.Sc. Chemistry - Semester III (M.Sc. 2-years Program)**  
**Advanced Coordination Chemistry & Inorganic Reaction Mechanism**  
**Subject Code: CH601B1**

**(Credits: Theory-04)**

**Course Objectives**

Detailed understanding of CFT, LFT & MOT and their use in inorganic complexes. Understanding of various types of transitions and their interpretation. Introduction to reaction mechanism with examples. Understanding of special organometallic reactions.

**Course/Learning Outcome**

At the end of the course, the students will be able to:

1. Understanding of VBT, CFT, CFSE and their applications. Influence on distortion of spectra
2. Understanding fundamentals of molecular orbital theory and ligand field theory.
3. Ability to predict electronic transitions and interpret electronic spectra of transition metal complexes.
4. Understanding fundamentals of reaction mechanism & electron transfer reaction mechanism
5. Understand the importance of use of organometallic catalysts in different reactions & bonding in carbonyl complexes

**Module I**

**Nature of Metal Ligand Bonding in Complex Compounds** (10 Lectures)

Valence bond theory in octahedral, tetrahedral & square planar complexes, Crystal field theory (CFT), Splitting of d orbital in octahedral, Tetrahedral and square planar complex, Crystal Field Stabilization Energy (CFSE), Determination of  $\Delta_o$  (CFSE) for various configurations, factors influence the magnitude of  $\Delta_o$ , application of CFT, Jahn-Teller Distortion.

**Module II**

**Molecular Orbital Theory & Ligand Field Theory** (10 Lectures)

Molecular Orbital Theory (MOT), Molecular orbital approach to bonding in octahedral complexes, Energy order of orbitals and their filling with electrons, sigma bonding in octahedral and tetrahedral complexes,  $\pi$  bonding in octahedral complexes,  $\pi$  donor ligands (CTLM),  $\pi$  acceptor ligands (CTML), Orgel diagram, Tanabe-Sugano diagram, Ligand field theory, Nephelauxetic effect, evidence for covalent bonding in complexes: adsorption spectra and Electron paramagnetic resonance spectra. (EPR).

**Module III**

**Electronic Spectra of Transition Metal Complexes** (10 Lectures)

Microstate calculation, L-S coupling, coupling of orbital angular momenta, coupling of spin angular momenta, selection rule, calculation of ground state terms, Hund's rule, Mulliken symbol in octahedral field, Orgel diagram, Spectra of  $d^1$  and  $d^9$ ,  $d^2$  and  $d^8$ ,  $d^3$  and  $d^7$  in octahedral & tetrahedral complex,  $d^5$  and  $d^8$  spectra in octahedral complex. Microstate table and its use in predicting electronic transitions.

## Module IV

### Inorganic Reaction Mechanism

(09 Lectures)

Substitution and electron transfer reaction - Nucleophilic Substitution in square planar and octahedral complexes, Kinetics, Associative- Dissociative mechanisms, Trans effect, influence of acids-bases and other factors in reactions. Outer sphere and Inner sphere electron transfer in octahedral complexes, electron transfer and its application, kinetic and thermodynamic stability, Labile and inert complexes.

## Module V

### Special Organometallics & Bonding in Carbonyl Complexes

(09 Lectures)

Bonding in Carbonyl complexes, Special organometallics - Reaction and applications, Suzuki reactions, Stille reaction, Negishi Cross coupling, Heck reactions, Buchwald-Hartwig Reaction, Sonogashira reactions.

### Textbooks/Reference Books

1. Advanced Inorganic chemistry - F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann.
2. Inorganic Chemistry, Principles of Structure and Reactivity - James E. Huheey, Ellen A. Keiter, Richard L. Keiter.
3. Inorganic Chemistry - Atkins and Shriver.
4. Inorganic Chemistry – G. L. Miessler, P. J. Fischer & D. A. Tarr.

**M.Sc. Chemistry - Semester III (M.Sc. 2-years Program)**  
**Concepts in Organic Synthesis**  
**Subject Code: CH602B1**

**(Credits: Theory-04)**

**Course Objective**

This course will introduce the basic idea of Pericyclic reactions, Organic photochemistry, concepts of oxidation-reduction, heterocyclic chemistry and introduction of natural products.

**Course/Learning Outcome:**

CO1: Ability to identify and deduce mechanisms of various types of pericyclic and photochemical reactions.

CO 2: In-depth understanding of solid-state chemistry of peptides and its applications.

CO 3: In-depth understanding of catalysis in chemistry and its applications.

CO 4: Ability to identify and apply oxidation-reduction reactions in synthesis.

CO 5: In-depth knowledge of heterocyclic chemistry and its applications.

**Module I**

**Pericyclic Reactions**

(09 Lectures)

Postulates and derivation of the kinetic gas equation; collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity, calculation of  $\sigma$  from  $\eta$ ; variation of viscosity with temperature and pressure. Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy.

**Module II**

**Organic Photochemistry**

(08 Lectures)

Principle, photochemical energy, orbital symmetry consideration related photochemical reactions, electronic oxidation, excited state of organic molecule, modes of dissipation of energy, energy transfer, quantum yield, cis-trans isomerization, photo-fragmentation reaction (Barton, Hofmann-Löffler-Freytag), Norrish type (I) & (II) reactions, Paterno Buchi reaction, Photo reduction, di- $\pi$  methane, aza-di- $\pi$  methane rearrangement, photocyclo addition, Photo chemistry of  $\alpha$ ,  $\beta$ -unsaturated ketones, reaction with singlet oxygen, application of photochemical methods in organic synthesis (Tranylcypromine).

**Module - III**

**Oxidation & Reduction Reactions**

(08+07 Lectures)

**Reduction:** Reduction of C-C multiple bond and carbon-hetero multiple bond: Catalytic hydrogenation (both hydrogen and hydride transfer mechanism), Electrochemical reduction at a low overvoltage electrode, Reduction by metal hydrides and alkoxides (LAH, DIBAL-H,  $\text{Bu}_3\text{SnH}$ ), Borane and borohydride,  $\text{R}_3\text{SiH}$ , Reduction by dissolving metals, Stereo/enantioselectivity reductions (Chiral Boranes, Corey-Bakshi-Shibata).

Oxidation: Formation of C=C by dehydrogenation – dehydrogenation by selenium dioxide, Formation of alcohols from hydrocarbons, Jones reagent, Sarett's reagent, PCC, Swern oxidation, MnO<sub>2</sub>, IBX, MPV, Pb(OAc)<sub>4</sub>, NaIO<sub>4</sub>, HIO<sub>4</sub>, Dakin reaction, O<sub>3</sub>, m-CPBA, VO(acac)<sub>2</sub>, Sharpless asymmetric epoxidation.

#### Module - IV

##### Heterocyclic Chemistry (07 Lectures)

Introduction, classification, nomenclature, reactions of aziridine, oxirane, thiirane, oxaziridine, azetidine, azetidinone, oxetane, oxetanone, thietane, pyrrole, furan, thiophene, 1,2- and 1,3-azoles, triazoles, pyridine, diazines, triazine and their oxy-derivatives. Application of heterocycles in various emerging fields - especially in medicine, and natural products.

#### Module - V

##### Catalysis (06 Lectures)

Heterogeneous catalysis: Preparation of catalyst and applications heterogeneous catalysis in synthesis of drugs. Homogenous catalysis: Introduction, hydrogenation, Wilkinson catalysts, Ziegler-Natta catalysts, applications of homogeneous catalysis in synthesis of drugs.

##### Chemistry of Peptides (03 Lectures)

Principle and methods of solid phase peptide synthesis, activation procedures, coupling reactions, protection, deprotection and cleavage from resin.

#### Textbooks/Reference Books

1. Finar, I. L., Organic Chemistry, vol. I & II (ELBS).
2. Advanced Organic Chemistry by J. March, Wiley Interscience.
3. Organic Chemistry by Morrison and Boyd
4. Reaction mechanism in organic chemistry by Mukhreji & Singh
5. Design of organic synthesis by M. Taylor
6. Stereochemistry of Carbon Compounds – E. L. Eliel
7. Organic Chemistry – J. Clayden; N. Greeves; S. Warren; P. Wothers
8. Modern Methods in Organic Synthesis – W. Carruthers

**M.Sc. Chemistry - Semester III (M.Sc. 2-years Program)**  
**Chemical Dynamics and Electrochemistry**  
**Subject Code: CH603B1**

**(Credits: Theory- 04)**

**Course Objectives**

The objective behind studying Chemical dynamics and electrochemistry is to present theories and applications related to the various chemical reactions and to update the students with the latest developments in the above field.

**Course/Learning Outcomes (CO)**

CO1: To impart basic knowledge of Chemical Kinetics of Collision theory and the activated complex theory. To understand the mechanisms of unimolecular reactions.

CO2: To understand the chemistry of Complex reactions, consecutive reactions, chain reactions, oscillatory, Thermal & photochemical chain reactions. To understand the kinetics of fast reactions.

CO3: To acquire knowledge on electrolytic conductance and the principles of Debye-Huckel model of ion-ion interactions and its verification.

CO4: To understand the theory of Activity and activity coefficients in electrolytic solutions.

CO5: To impart knowledge on electrified interface and Approximate models of electrified interface.

**Module I**

**Chemical Kinetics-I** (12 Lectures)

Arrhenius equations, concept of transition state, transition state theory-mechanism, collision theory, steric factor, comparison between collision & Transition state theory, Potential energy surface, thermodynamic treatment of reaction rates, Energy of activation, volume of activation, Series & Parallel reactions, Equilibrium from kinetic point of view, Kinetic isotope effect and solvent isotope effect, treatment of unimolecular reactions-Lindemann's theory, Hinshelwood's theory.

**Module II**

**Chemical Kinetics-II** (10 Lectures)

Complex reactions, consecutive reactions, chain reactions and oscillatory, Thermal & photochemical chain reaction between  $H_2$  &  $Cl_2$  and  $H_2$  &  $Br_2$ , Influence of dielectric constant and ionic strength on reaction rate, linear free energy relationship, effect of substituents, fast reactions. Luminescence and energy transfer process, study by stop flow techniques, relaxation method.

**Module III**

**Electrochemistry** (08 Lectures)

Electrolytic Conductance- Theory of electrolytic conductance: Degree of dissociation, time of relaxation, Mechanism of electrolytic conductance. Dispersion of conductance: Debye-Falkenhagen effect and Wien effect. Onsager equation, Debye – Huckel theory of dilute electrolytes, derivation of Debye-Huckel conductance equations for dilute solution, Verification of Debye – Huckel theory.

## Module IV

### Free Energy and Activity (10 Lectures)

Activity & activity coefficients, its method of determination, Forms of activity coefficients and significance. Significance of the Degree of Dissociation- ion-pairs and factors affecting ion pair formation. Activities of Electrolytes and Values of Activity Coefficients. Limiting & extended Debye-Huckel equation for activity coefficient, The Huckel and Bronsted Equations.

## Module V

### Electrified Interface (08 Lectures)

Approximate models of electrified interface: Helmholtz Compact layer model, Gouy-Chapman diffuse layer model and Stern Model.

### Textbooks/Reference Books

1. Laidler, K. J. Chemical Kinetics 3rd Ed., Pearsons (2011)
2. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006)
3. McQuarrie, D. A. & Simon, J. D. Physical Chemistry: A Molecular Approach 3rd Ed., Univ. Science Books (2001)
4. Bockris, J. O' M. & Reddy, A. K. N. Modern Electrochemistry 1: Ionics 2nd Ed., Springer (1998).
5. Bockris, J. O' M. & Reddy, A. K. N. Modern Electrochemistry 2B: Electroics in Chemistry, Engineering, Biology and Environmental Science 2nd Ed., Springer (2001)
6. Bockris, J. O' M., Reddy, A. K. N. & Gamboa-Aldeco, M. E. Modern Electrochemistry 2A: Fundamentals of Electroics 2nd Ed., Springer (2001).
7. Brett, C. M. A. & Brett, A. M. O. Electrochemistry, Oxford University Press (1993)
8. Moore, W. J. Physical Chemistry 4th Ed. Prentice-Hall (1972).
9. Electrochemistry, S. Glasstone

**M.Sc. Chemistry - Semester III (M.Sc. 2-years Program)**  
**Photoinorganic Chemistry**  
**Subject Code: CH601B3**

**(Credits: Theory- 04)**

**Course Objective**

Introduction to photochemistry, concepts, application and industrial use.

**Course/Learning Outcome**

CO1: In- depth understanding of photochemical Laws, Ability to explain various photophysical process taking place in excited state and factors influencing them.

CO2: Ability to identify and explain photophysical kinetics of excited state in gaseous and liquid state and electron transfer process.

CO3: In-depth understanding of photo-reduction and related reactions.

CO4: Ability to identify various types of photochemical reactions and its application.

CO5: In-depth understanding of photochemical reactions in biological processes and its explanation using model systems.

**Module I**

**Introduction to Inorganic Photochemistry** (08 Lectures)

Importance of photochemistry, Laws of photochemistry, quantum yield, thermochemical and photochemical reactions, photochemical equilibrium, photochemistry and spectroscopy, Charge transfer and charge transfer to solvent transition. Photophysical process in electronically excited molecules - Jablonski diagram, radiation-less transitions, selection rules. Fluorescence emission, fluorescence and structure. Triplet states and phosphorescence emission.

**Module II**

**Collisions in Solution & Kinetics** (08 Lectures)

Photophysical kinetics of unimolecular process, delayed fluorescence, effect of temperature on emission processes. Photophysical kinetics of bimolecular process – kinetic and optical collisions, bimolecular collisions in gases and vapours. collisions in solution, kinetics of collisional quenching: Stern-Volmer equation, deviations, Excimer and excited state dimers, exciplex formation and decay. electronic energy transfer mechanism.

**Module III**

**Photo Reduction and Related Reactions** (08 Lectures)

Photo reduction and related reactions, Photo oxidation and photo oxygenation, Chemiluminescence, Photosensitization. Photochemical reactions; substitution, decomposition and fragmentation, rearrangement, and redox reactions.

**Module IV**

**Photochemical Reaction** (08 Lectures)

Photochemical reaction between anthracene and carbon tetrachloride, determinations of quantum yield of reaction, factors affecting the quantum yield of reaction, Photoreactive state of anthracene.

## **Module V**

### **Selective Inorganic Photochemistry**

(08 Lectures)

Selective inorganic photochemistry using laser beams. Inorganic photochemistry in biological processes and their model studies- Mutagenic effect of radiation, Photosynthesis.

### **Texts Books/Reference Books**

1. Organometallic Photochemistry, Academic Press, 1979 – G. L. Geoffrey & M. S. Wrighton
2. Fundamentals of Photochemistry, Wiley Eastern, 1978 – K. K. Rohatagi-Mukherjee
3. Inorganic and Organometallic photochemistry, ACS Pub., 1978 – M. S. Wrifhron
4. Photochemistry of Co-ordination compounds, Academic Press, 1970 – V. Balzani and V. Carassiti

**M.Sc. Chemistry - Semester III (M.Sc. 2-years Program)**  
**Synthetic Organic Chemistry**  
**Subject Code: CH602B3**

**(Credits: Theory- 04)**

**Course Objective**

This course will discuss the use of various organometallic compounds in organic synthesis, chemistry of B, Si, P, S and Sn. Moreover, the role of transition metal complexes in organic synthesis and asymmetric synthesis will be covered in this subject area. Knowledge on retrosynthesis, protection & deprotection of functional group and application of spectroscopy for the determination of organic structures will be provided to make clear understanding among students about organic synthesis.

**Course/Learning Outcome**

CO1: Explain and identify organometallic and their uses in organic synthesis.

CO2: Explain and identify organometalloid and their uses in organic synthesis.

CO3: Ability to demonstrate knowledge of asymmetric synthesis.

CO4: Design retro-synthetic strategies independently for compounds of moderate complexity.

CO5: Explain and solve how to project and deprotect functional groups during organic synthesis.

**Module I**

**Organometallics of Group I & II and Organometalloids**

(16 Lectures)

Organometallic compound of Gr I and II metals: preparation and properties, reaction with carbonyl and alkylating agents.

Boron Chemistry: Organoboranes- preparation and properties of organoborane reagents e.g.  $\text{RBH}_2$ ,  $\text{R}_2\text{BH}$ ,  $\text{R}_3\text{B}$ , 9-BBN, Thexyl borane, cyclohexyl borane, Hydroboration-mechanism, stereo and regioselectivity, uses in synthesis of primary, secondary tertiary alcohols, aldehydes, ketones, alkenes. Synthesis of E, E; E, Z; Z, Z dienes and alkynes. Allyl boranes- synthesis, mechanism and uses.

Phosphorous Chemistry: Preparation & properties of  $\text{PPh}_3$ ,  $\text{P}(\text{OEt})_3$ ,  $\text{POCl}_3$ ,  $\text{PBr}_3$ ,  $\text{PCl}_5$ , etc. Wittig-Horner reaction, Mitsunobu reaction, Staudinger reaction, Vilsmeier-Haack reaction, Corey-Winter reaction.

Sulphur Chemistry: Reaction with  $\text{CS}_2$ ,  $\text{SO}_2$ ,  $\text{SO}_3$ ,  $\text{SOCl}_2$ ,  $\text{SO}_2\text{Cl}_2$ ,  $\text{PhSNa}$ , 1,3-dithiane, DMSO,  $\text{RSCl}$ , sulphur ylide in organic synthesis.

**Module II**

**Transitional Metals Complexes in Organic Synthesis**

(10 Lectures)

Introduction, oxidation states of transition metals, 16-18 rule, dissociation, association, insertion, oxidative addition, reductive elimination of transition metal.

Organocopper Intermediates: Preparation and structure, reaction involving organocopper.

Organopalladium in Organic Synthesis: Heck arylation, allylic activation, carbonylation, wacker oxidation, isomerization formation N-aryl and N-alkyl bond transmetalation.

Organonickels: Coupling carboxylation, carbonylation. Reaction involving rhodium and ruthenium.

### Module III

#### Asymmetric Synthesis

(10 Lectures)

Stereoselective and stereospecific reactions, prochirality, Chemo-, regio-, diastereo- and enantio-controlled approaches; Chirality transfer, Asymmetric inductions; Chiral pools, Chiral auxiliaries, Chiral reagents and catalysts, and templates.

Asymmetric Oxidations: dihydroxylation, aminohydroxylation, Asymmetric reduction reactions: Reduction of ketones, imines and olefins (use of BINAP).

Asymmetric C-C Bond Forming Reaction: Simmons-Smith reaction, Mukaiyama aldol reaction, Shibasaki bi-metallic catalyst system.

### Module IV

#### Retrosynthesis

(06 Lectures)

Basic principles and terminology of retrosynthesis, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions.

### Module V

#### Protection & Deprotection of Functional Group

(06 Lectures)

Protecting Groups: Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection; illustration of protection and deprotection in synthesis.

#### Texts Books/Reference Books

1. Advanced Organic Chemistry by J. March, Wiley Interscience.
2. Organic Chemistry by J. Clayden; N. Greeves; S. Warren; P. Wothers
3. Principles of Organic Synthesis by R. O. C. Norman
4. Modern methods in organic synthesis by W. Carruthers and I. Coldham
5. Advanced Organic Chemistry - Part B: Reactions & Synthesis by F. A. Carey & R. J. Sundberg
6. Chiron approach in organic synthesis by S. Hanessian (Relevant chapters for Chirons)
7. Asymmetric Reactions and Processes in Chemistry: Ernest L. Eliel
8. Comprehensive Organic Transformations: A Guide to Functional Group Preparations, 2nd edition (1999) by Richard C. Larock.
9. Protective Groups in Organic Synthesis, 3rd edition (1999) by Theodora W. Greene and Peter G. M. Wuts

**M.Sc. Chemistry - Semester III (M.Sc. 2-years Program)**  
**Advanced Physical Chemistry**  
**Subject Code: CH603B3**

**(Credits: Theory- 04)**

**Course Objective**

To introduce the concepts of statistical mechanics and thermodynamics as it relates the macroscopic properties of a system to the properties of the atoms and molecules which constitutes a system.

**Course/Learning Outcome**

CO1: Able to find the connection between statistics and thermodynamics. and differentiate between classical statistics and quantum statistics.

CO2: Able to account for the physical interpretation of partition functions and be able to calculate thermodynamic properties of model systems with using Boltzmann, Fermi-Dirac and Bose-Einstein statistics.

CO3: Ability to understand basics of Quantum Statistics.

CO4: Able to understand process of aggregation of amphiphilic molecules and their industrial application.

CO5: Ability to determine surfactant aggregation using experimental techniques.

**Module I**

**Statistical Thermodynamics** (10 Lectures)

Basic Statistical Thermodynamic, Phase space, Assembly & Ensemble, canonical form, statistical equilibrium & thermodynamic probability, Maxwell Boltzmann statistics.

**Module II**

**Partition Function** (10 Lectures)

Partition function and its types – Translational, Rotational, Vibrational, and Electronic partition function. Relations of partition function with thermodynamic functions such as internal energy, heat capacity, Entropy & probability, heat content, work function 'A', Gibb's free energy, heat content and third law of thermodynamics and equilibrium constant from partition functions.

**Module III**

**Quantum Statistics** (08 Lectures)

Quantum Statistics- Bose- Einstein & Fermi Dirac statistics and its application, Theories of specific heat of solids classical and Einstein treatment

**Module IV**

**Surfactants** (10 Lectures)

Introduction: Characteristic features of surfactants and amphiphiles. Various types of amphiphiles. Self-assembly and the critical packing parameter. Factors affecting self-aggregation.

**Module V**

**Experimental Methods for Detection of Self-aggregation** (10 Lectures)

Experimental methods for detection of self-aggregation. Thermodynamic parameters of amphiphilic aggregation.

Vesicles, Types of vesicles, Gel-to-liquid crystalline phase transition. Differential Scanning Calorimetry studies. Lichtenberg three stage model.

**Texts Books/Reference Books**

1. Surfactants and Interfacial Phenomena – Milton J. Rosen. John Wiley & Sons, Inc
2. Surfactant Aggregation – J. H. Client. Springer
3. Thermodynamics-A core course – Srivastava, Saha & Jain.
4. Statistical Thermodynamics – M. C. Gupta
5. Fundamentals of classical and Statistical Thermodynamics - B. N. Roy
6. Classical and Statistical Thermodynamics - A. H. Carter

**M.Sc. Chemistry - Semester III (M.Sc. 2-years Program)**  
**Inorganic Chemistry Lab**  
**Subject Code: CH601B4**

**(Credits: Lab-03)**

**Course Objectives**

To gain experience in synthetic techniques and interpretation of the spectra based on concepts learned in theory

**Course/Learning Outcome**

CO1: Enable to synthesize different first row transition metal complexes, their purification and crystallization.

CO2: Enable to determine percentage of yield of the products and to characterize physical properties.

CO3: Enable to carry out UV-vis spectroscopic studies of the prepared complexes.

CO4: Enable to carry out FTIR spectroscopic studies of the prepared complexes.

CO5: Enable to analyse UV-vis and FTIR spectral data (Molar extinction coefficient, identification of d-d transition and charge transfer).

**List of Experiments**

1. Synthesis of first row transition metal complexes and their purification (minimum of 10 complexes).
2. UV-vis spectroscopic studies of the prepared complexes:
  - c) Role of metal ions
  - d) Influence of ligands
  - c) Total interpretation of spectra and correlation with CFT

**Textbooks/Reference Books**

1. Co-ordination Chemistry Reviews
2. Journal of Chemical Education
3. Inorganic Chemistry, Principles of Structure and Reactivity – James E. Huheey, Ellen A. Keiter, Richard L. Keiter

**M.Sc. Chemistry - Semester III (M.Sc. 2-years Program)**  
**Organic Chemistry Lab**  
**Subject Code: CH602B4**

**(Credits: Lab-03)**

**Course Objectives**

This course will help provide hand on experiences of various techniques adopted in organic synthesis. Students will be able to handle various routine techniques used during organic synthesis in laboratory.

**Course/Learning Outcome**

CO1: Learn and apply techniques used purification of organic solvent.

CO2: Apply difference chromatographic techniques used in purification of organic molecules.

CO3: Apply crystallization techniques for purification of organic molecule.

CO4: Explain and estimate the concentration of organic molecule through redox titration.

CO5: Apply various green synthesis techniques for preparation of organic molecule/derivatives.

**List of Experiments**

1. Purification of organic molecules/solvents through normal distillation, distillation under reduced pressure,
2. Hand on experience on thin layer chromatography (TLC) / PTLC, crystallization and Column chromatography for separation/purification of organic molecule.
2. Estimation of Glucose and phenol or acetone through redox reaction.
3. Some Green Organic synthesis
  - (e) Bromination
  - (f) Acetylation
  - (g) Nitration
  - (h) Some name reactions
4. Organic synthesis in solid support. (with or without microwave irradiation)

**Textbooks/Reference Books**

1. Vogel's textbook of practical organic chemistry - Furniss Hannaford Smith, Tatchell
2. Monograph on Green Chemistry – Laboratory Experiment - Green Chemistry task force committee, DS

**M.Sc. Chemistry - Semester III (M.Sc. 2-years Program)**  
**Project Based Learning**  
**Subject Code: CH601B5**

**(Credits: Project-01)**

**M.Sc. Chemistry - Semester IV (M.Sc. 2-years Program)**  
**Bio-inorganic Chemistry**  
**Subject Code: CH604B1**

**(Credit: Theory-03)**

**Course Objective**

The students will acquire in-depth knowledge of role of transition metal ions and its complexes in different biological processes and their chemistry in treatment of different diseases.

**Course/Learning Outcome**

CO1: Understanding of basic reactions in the biological systems and storage & transport of metabolic energy.

CO2: Ability to understand ion transport across the biological membrane. To know the working of sodium ion pump.

CO3: In-depth knowledge of biological redox reactions, their importance and dioxygen in biological systems.

CO4: In-depth Knowledge of metalloproteins in biological system and their active site structures.

CO5: Knowledge of metalloenzymes and their applications in biological systems.

**Module I**

**Basic Biological Inorganic Reaction** (08 Lectures)

a) Basic reactions in the biological system and the roles of metal ions. Metal complexes in medicine- cisplatin, auranofin.

b) Metal – nucleic acid interactions - Metal ion interaction with Nucleosides & Nucleotides, Metal ion interaction with DNA, Metal ion interaction with RNA.

c) ATP =ADP Interconversion, Creatine- Phosphocreatine interconversion, phosphate transfer and its activation by metal ions.

**Module II**

**Transport Across Biological Membrane** (08 Lectures)

Transport Across Biological membrane – Ionophores as metal ion carriers- cyclic natural ionophores, open chain carboxylic acid ionophores & other ionophores. Active transport across the membrane,  $\text{Na}^+/\text{K}^+$  transporting AT Pase,  $\text{Na}^+$  ion pump.

**Module III**

**Biological Redox Reaction** (08 Lectures)

Biological Redox Reaction- Electron transport proteins – Ferredoxins, Cytochromes. Energetics of electron transport in the respiratory chain, Photosynthesis.

Dioxygen in Biological system- Reactions of molecular oxygen, Activation of Dioxygen Molecule in Transition metal Dioxygen complexes.

**Module IV**

**Metalloproteins** (08 Lectures)

Oxygen carrying proteins- Haemoglobin & Myoglobin, Hemerythrin, Hemocyanin, cooperatively in haemoglobin, Bohr effect, Blood Substitute.

Model system- Synthetic oxygen carriers-

(i) Porphyrin Derivatives,

(ii) Cobalt (II) Dioxygen complexes

(iii) Iridium (II) Dioxygen complexes (Vaska's complexes)

(iv) Platinum group metal dioxygen complexes.

## Module V

### **Metalloenzymes**

(08 Lectures)

Redox enzymes- Molybdenum containing enzymes, Iron containing enzymes, Copper containing enzymes, Zinc containing enzymes.

Hydrolytic Enzyme-Carboxy peptidase, carbonic anhydrase

Vitamins & co-enzymes.

### **Textbooks/Reference Books**

1. Biochemistry – L. Stryer
2. Principles of Bioinorganic chemistry – S. J. Lippard and J. M. Berg
3. Inorganic Biochemistry – G. L. Eichhorn
4. Elements of Bioinorganic Chemistry – G. N. Mukherjee, A. Das
5. Bioorganic, Bioinorganic and Supramolecular Chemistry – P. S. Kalsi, J. P. Kalsi

**M.Sc. Chemistry - Semester IV (M.Sc. 2-years Program)**  
**Solid State Chemistry and Interface Science**  
**Subject Code: CH605B1**

**(Credit: Theory-03)**

**Course Objective**

The course introduces the concept of molecular arrangements within crystalline solids followed by the aggregation of specific molecules into colloids and its applications

**Course/Learning Outcome**

CO1: Able to understand basic concept of crystal structure, its defect and its application to explain electrical properties of the solid material.

CO2: Able to describe the fundamental concept of Band Theory.

CO3: Understand surface chemistry of Adsorption

CO4: Ability to understand the basics of colloids and their applications.

CO5: Understand the various processes of Photochemistry.

**Module I**

**Solid State Chemistry** (08 Lectures)

Unit cell, Miller indices, Bravais lattice, Bragg's equation, crystal structure analysis, Structure of NaCl, KCl, and Zinc Blende, Types of defects in solids and its influence on electrical properties of solids.

**Module II**

**Band Theory** (08 Lectures)

Band theory and its application, Insulators & semiconductors and its types & preparation, superconductor and its application, Macromolecules: concept molecular mass, its determination.

**Module III**

**Surface chemistry** (08 Lectures)

Adsorption of gases on solids, Freundlich's adsorption isotherm, Langmuir adsorption isotherm, Gibb's adsorption equations, BET Application of Adsorption.

**Module IV**

**Colloids** (08 Lectures)

Association colloids, Preparation of colloidal sol and application of colloidal Science application, Emulsion and micro emulsion formation and thermodynamics application (detergency), Solubilization of surfactant solution Donnan Membrane equilibrium.

**Module V**

**Photochemistry** (08 Lectures)

Einstein law of Photochemical equivalence, quantum yield, primary and secondary processes, Photoelectric effect, Latent Image, Elementary idea of laser and its application.

**Texts Books/Reference Books**

1. Physical Chemistry of Surface – A. W. Adamson & A. Gast
2. Solid State chemistry and Its Applications-Anthony R. West
3. Basic Solid State Chemistry – A. R. West
4. Solid State Chemistry – Kettal
5. Applied colloid and surface chemistry – R. Pashley
6. Colloids and Interface with Surfactants and Polymer – James W Goodwin

**M.Sc. Chemistry - Semester IV (M.Sc. 2-years Program)**  
**Group Theory – A Chemist Approach**  
**Subject Code: CH606B1**

**(Credit: Theory-03)**

**Course Objective**

To provide basic understanding of group theory and its application in chemistry. The course will help students to clear the concept of spectroscopy.

**Course/Learning Outcome**

CO1: Ability to identify the symmetry elements and symmetry operation in molecules.

CO2: Ability to identify point group, group multiplication table, subgroups and various groups.

CO3: Ability to make transformation matrix for various symmetry elements.

CO4: Ability to make the character representation of a point group on different basis sets.

CO5: Able to construct character table and apply them to find various properties of molecules.

**Module I**

**Symmetry Elements and Symmetry Operations** (12 Lectures)

Introduction, importance of symmetry, geometry of molecule through VSEPR theory, different symmetry elements, symmetry operation of each symmetry element, horizontal plane, vertical plane, dihedral plane, associated operation of  $S_n$  axis, finding out symmetry elements present in  $AB_2$  (linear and bent),  $AB_3$  (Planar and pyramidal),  $AB_4$  (tetrahedral and planar),  $AB_5$  (planar, trigonal bipyramidal, square pyramidal),  $AB_6$  (planar, octahedral), spiro, cycloalkane [especially cyclohexane (chair, boat)], conformations of ethane (staggered, eclipsed), alkene, alkyne, ferrocene etc, product of symmetry operations, commutative symmetry operation.

**Module II**

**Symmetry Elements and Point Groups** (10 Lectures)

Mathematical rules for the formation of a group, flow chart for determination of point group, symmetry elements present in a point groups, variation of symmetry elements and point group by substitution, order of a group, group multiplication table for a  $C_s$ ,  $C_i$ ,  $C_n$ ,  $C_{nv}$ ,  $C_{nh}$  etc, conjugate elements and classes of different point groups, subgroups of a point group, Isomorphic group, Abelian group, Symmetry number, application of point group on optical activity and dipole moment.

**Module III**

**Matrix Representation of Symmetry Operations** (06 Lectures)

Definition, order, matrix multiplication and addition, transpose of a matrix, inverse of a matrix, Solutions of linear equations by matrix method, transformation matrices for i) identity ii) plane of symmetry iii) centre of symmetry iv) axis of symmetry v) improper axis of symmetry, transformation matrix for  $S_n$  axis.

## Module IV

### Representation of Point Groups

(06 Lectures)

Characteristic of matrix representation, character representation of a point group, method for deriving matrix representations on different basis set, method to directly arrive character representation, classification of representations

## Module V

### Character Table

(10 Lectures)

The great orthogonality theorem, Application of the orthogonality theorem, construction of character tables, Character table of various point group, Mullikan symbols for IR's, Determination of symmetry species for translations and rotations. IR active and Raman active vibrations.

### Texts Books/Reference Books

1. Chemical Applications of Group Theory – F. A. Cotton
2. Molecular Spectroscopy – D. J. Willock
3. Symmetry and Spectroscopy of Molecules – K. V. Reddy
4. A Simple Approach to Group Theory in Chemistry – S. Swarnalakshmi, T. Saroja, R M Ezhilarasi

**M.Sc. Chemistry - Semester IV (M.Sc. 2-years Program)**  
**Quantum Chemistry-II**  
**Subject Code: CH607B1**

**(Credit: Theory-03)**

**Course Objective**

The course aims to introduce students to an advanced state of quantum chemistry where the students will apply the basic principles and model systems of quantum mechanics to real systems with the help of approximation methods

**Course/Learning Outcome:** On successful completion of this course students would be able to  
CO1: Apply Variation method to solve the wave functions of common model systems in quantum chemistry.  
CO2: Apply perturbation theory to solve quantum mechanical problems.  
CO3: Elucidate the wave functions of He and other multi-electronic systems using approximation techniques.  
CO4: Correlate the Born Oppenheimer approximation and MOT with the PE curve of molecules.  
CO5: Explain chemical bonding using VB and HMO theories.

**Module I**

**Approximation Methods** (08 Lectures)  
Variation method, Linear and nonlinear variation functions and its application in particle in a box, simple harmonic oscillator and hydrogen atom systems.

**Module II**

**Perturbation Method** (08 Lectures)  
First and second order corrections and its application in particle in a box, simple harmonic oscillator and hydrogen atom systems.

**Module III**

**Helium Atom and Other Multielectronic Systems** (10 Lectures)  
Application to two electron system.: electron spin, spin orbital, Pauli exclusion rule, columbic and exchange energies. Excited state of He atom, symmetric and antisymmetric wave functions. Multielectron atoms, determinantal form of the wave function, self-consistent field approximation, Hartree-Fock Self Consistent field theory, Slater type orbitals.

**Module IV**

**Molecular Systems** (08 Lectures)  
Separation of electronic and nuclear motions treatment of homonuclear and heteronuclear diatomic molecules- the Born Oppenheimer approximation, MO theory, LCAO-MO approximation, MO's of  $H_2^+$  and  $H_2$  molecule.

## Module V

### Valence Bond Theory and Semi Empirical Methods

(10 Lectures)

Valence bond theory, Heitler-London theory, electron density distributions, the Ab-initio calculations semiempirical methods. Huckel theory for linear and cyclic conjugated systems; Applications to simple  $\pi$  systems: Ethylene, vinyl, cyclopropenyl.

### Text Books/Reference Books

1. Quantum Chemistry – Levine
2. Quantum Chemistry – R K Prasad
3. Molecular Quantum Mechanics – P. W. Atkins
4. Quantum Chemistry – Pauling & Wilson
5. Quantum Chemistry – F. L. Pilar
6. Quantum Chemistry – McQuarrie
7. Quantum Chemistry – Eyring, Walter and Kimball

**M.Sc. Chemistry - Semester IV (M.Sc. 2-years Program)**  
**Chemistry of Nanomaterials**  
**Subject Code: CH604B3**

**(Credit: Theory-04)**

**Course Objective**

The course introduces the concept of nano science, specifically nano material chemistry and its applications.

**Course/Learning Outcome**

CO1: Explain and identify basic aspects of nanomaterials.

CO2: Ability to generate new methods for synthesis of nanomaterials.

CO3: Demonstrate and identify porous and carbon materials.

CO4: Demonstrate and identify various experimental techniques and characterizations of nanomaterials.

CO5: Apply nanomaterials in various fields of chemistry.

**Module - I**

**Basic Aspects at Nanoscale Materials** (10 Lectures)

Surface plasmon effect, semiconductor nanoparticles, quantum confinement, magic number in clusters, physical chemistry of solid surfaces and at the nanoscale, surface (electrostatic and steric stabilization), bottom-up synthesis approach, nucleation theory, growth mechanisms and its control, Ostwald ripening, Fundamentals of film growth, nucleation process in film formation.

**Module - II**

**Nanomaterial Synthesis** (10 Lectures)

Chemical routes, electrochemical methods and vapor growth. thin films methods, chemical vapor deposition, physical vapor deposition (sputtering, laser ablation) and Langmuir-Blodgett growth. mechanical methods: ball milling and mechanical attrition. sol-gel methods, bioinspired synthesis.

**Module - III**

**Porous and Carbon Materials** (10 Lectures)

Micro and mesoporous materials: zeolites, porous silicon synthesis, formation mechanism, different applications Special nanomaterials: graphene, carbon nanotubes, fullerenes, nanowires.

**Module - IV**

**Overview of Different Characterization Techniques** (10 Lectures)

Overview of different experimental techniques for structural characterization of nanomaterials, Detail of the characterization techniques: X-ray diffractometry (XRD), Scherrer equation, crystal size measurement, transmission electron microscopy (TEM), bright-field and dark field imaging in TEM, selected area electron diffraction, scanning electron microscopy (SEM), BET surface area measurement, scanning tunneling microscopy (STM), atomic force microscopy (AFM).

## **Module - V**

### **Different Applications of Nanomaterials**

(08 Lectures)

Different applications of nanomaterials like in catalysis, environmental, biomedical, solar cells, electronic circuits, light emitting devices, data storage, biological tags, cancer treatments, drug delivery.

### **Texts Books/Reference Books**

1. Inorganic Materials Synthesis and fabrication – John N. Lalena. John Wiley and Sons.
2. Nanochemistry: A chemical approach to nanomaterials – Geoffrey A. Ozin and Andre C. Arsenault. RSC Publishing.

**M.Sc. Chemistry - Semester IV (M.Sc. 2-years Program)**  
**Supramolecular Chemistry**  
**Subject Code: CH605B3**

**(Credit: Theory-04)**

**Course Objective**

Introduction to concepts of Supramolecular chemistry, various routes of synthesis, its uses and future possible application.

**Course/Learning Outcome**

CO1: Understanding Host-Guest Chemistry, receptors & Macrocyclic effects.

CO2: Understanding of various intermolecular forces and its application in construction of supramolecules.

CO3: Understanding chemistry of formation of various supramolecular systems and their application.

CO4: Knowledge of self-assembly process in construction of supramolecules.

CO5: Understanding the role of coordination chemistry in construction of functional supramolecular materials.

**Module I**

**Introduction** (10 Lectures)

From molecular to supramolecular Chemistry, Factors leading to strong binding, H-bonding and stacking interaction, Host-Guest Chemistry, Development, Classification of Supramolecular Host-Guest Compounds, Receptors, Coordination and the Lock and Key analogy, Chelate and Macrocyclic effects.

**Module II**

**Nature of Supramolecular Interactions** (10 Lectures)

Ion-Ion, Ion-Dipole, Dipole-Dipole, Hydrogen Bonding, Cation- $\pi$  Interaction,  $\pi$ - $\pi$  Interaction, Hydrophobic effect, Van der Waals Bonding Interaction, Cooperativity, Allosteric Systems.

**Module III**

**Supramolecular Systems** (08 Lectures)

Crown ethers, Podands, Cryptands, Spherands, Lariat ethers, Bibrachial Lariat ethers. Introduction, Synthesis, Nomenclature, Solution behaviour and application in specific recognition process.

**Module IV**

**Supramolecular Assembly of Complex Architectures** (10 Lectures)

Novel Supramolecular Architectures – Catenanes, Rotaxanes, Knots, Cyclodextrins, Cyclophanes, Siderophores. Porphyrins and its Derivatives for construction of Supramolecular Assemblies.

## Module V

### Coordination Chemistry Based Approach for Functional Supramolecular Materials

(09 Lectures)

Weal Link Approach, General strategy of WLA, components of WLA, Hemilabile ligands, Ancillary ligands, Functional supramolecular systems, host-guest as molecular sensors, catalytic systems, multivalency and cooperativity, Self-Assembled Molecular Flasks.

#### Texts Books/Reference Books

1. Supramolecular Chemistry by J. W. Steed & J. L. Atwood, published – Wiley
2. Supramolecular Chemistry by J. M. Lehn, published – Wiley – VCH
3. Review Articles
  - a) Development of a Coordination Chemistry - Based Approach for Functional Supramolecular Structures–Account of Chemical Research, Vol.38, No.11, 825-837, 2005
  - b) Multivalency and Cooperativity in Supramolecular Chemistry– Account of Chemical Research Vol.38, No.9.,723-732,2005
  - c) Functional Molecular Flasks: New Properties and Reactions within Discrete, Self-Assembled Hosts– Angew Chem. Int. Ed., 48, 3418-3438, 2009

**M.Sc. Chemistry - Semester IV (M.Sc. 2-years Program)**  
**Medicinal Chemistry**  
**Subject Code: CH606B3**

**(Credit: Theory-04)**

**Course Objective**

This paper will introduce drug design and their synthetic approach. Moreover, Cell structure, Protein structure, Drug action, RNA, DNA, Prodrugs etc will also be discussed. This will also give the idea of various syntheses and applications of Antipyretic Analgesics, Antibacterial agents, Antibiotics, Anti-ulcer agents, Local - Anaesthetics, Anti-cancer agents and Antimalarial.

**Course/Learning Outcome**

CO1: In-depth understanding of mode of action of drugs.

CO2: Synthesis and ability to establish structure-activity relationships of various classes of drug.

CO3: Understanding the role and function of Antihistamines.

CO4: Expertise in synthesis and classifications of various classes of local Anaesthetics.

CO5: In-depth understanding of various classes of Antimalarial drugs.

**Module I**

**Introduction**

(12 Lectures)

Cell structure and Protein structure. Pharmacodynamic, pharmacokinetic (drug adsorption, distribution, metabolism, and elimination) and toxicological aspects of stereoisomers (Geometrical, optical, and conformational). Drug action at Proteins, Drug action at enzymes, competitive and non-competitive inhibitors, Drug action at receptors, the drug receptor, the drug receptor interaction. Stages of drug discovery, lead discovery, identification, validation, and diversity of drug targets. Structure-activity relationships: Strategies in drug design. QSAR and combinatorial synthesis. Optimization of drug-target interactions and access to drug targets.

**Antipyretic Analgesics**

(04 Lectures)

Aniline and p-Aminophenol – Paracetamol, Phenacetin, Acetanilide. Salicylic acid analogues – Aspirin, Salol. N-Aryl anthranilic acid -- Mefenamic acid, Meclofenamate sodium.

**Module II**

**Antibacterial Agents**

(06 Lectures)

The bacterial cell, Mechanisms of antibacterial action. Sulphonamides and Sulphones – Development of sulphonamides as drug – Prontosil, sulphapyridine. Sulphonamides for general infection – Sulphanilamide, Sulphapyridine, Sulfathiazole, Sulfadiazine. Sulphonamides for Urinary infections – Sulfacetamide. Sulphonamides for Intestinal Infections – Phthalyl sulfathiazole, Succinyl sulphathiazole. Sulphonamides for Local Infection – Sulfacetamide, Mafenide. Sulphones --- Dapsone.

**Antibiotics**

(04 Lectures)

The Penicillin, General introduction to  $\beta$ - lactam antibiotics – Cephalosporins, Chloramphenicol, Tetracyclines – structure action relativity.

**Module III**

**Local Anaesthetics**

(07 Lectures)

Esters – Ethyl p-aminobenzoate, Butamben, Procaine hydrochloride, Tetracaine hydrochloride. Piperidine or Tropone derivatives – Eucaine, Benzamine hydrochloride. Amides – Lignocaine,

Prilocaine, Mepivacaine hydrochloride, Pyrrocaine hydrochloride. Miscellaneous Type – Phenacaine hydrochloride, Eugenol, Mode of action of some selected local anesthetics.

#### **Module IV**

##### **Antihistamines**

(07 Lectures)

Histamine H1-receptor Antagonists – Aminoalkyl ethers, Ethylenediamines, Thiophene derivatives, Cyclic basic chain analogues. Histamine H2 Receptor blockers - Peptic ulcers, Histamine Cimetidine – a rational approach to drug design, Cimetidine, ranitidine, famotidine and nizatidine.

#### **Module V**

##### **Antimalarials**

(08 Lectures)

Prevention of malaria, malarial parasites, Plasmodia, and their life cycle. 4-aminoquinoline – Structure activity relationship, chloroquine, Sontoquine. 8-amonoquinolines – structure activity relationship, pamaquine, primaquine – synthesis, absorption, distribution and excretion, toxicity, uses, routes of administration and dosage. 9-Aminoacridines – Mepacrine hydrochloride, Pyrimidines – Pyrimethamine.

##### **Texts Books/Reference Books**

1. An Introduction to Medicinal Chemistry – Graham L. Patrick (Oxford)
2. Medicinal Chemistry – Ashutosh Kar

**M.Sc. Chemistry - Semester IV (M.Sc. 2-years Program)**  
**Research Project Work**  
**Subject Code: CH602B6**

**(Credit: Research Project Work-04)**

**Course Objective**

Each Faculty member will provide a research topic to the student(s) from current research area at beginning of 1<sup>st</sup> semester. Each research project topic is different from other. Research Students will perform their research in chemistry lab from 1<sup>st</sup> semester. Students will get an exposure about the research in chemistry.