



**MANAV RACHNA  
UNIVERSITY**   
Declared as State Private University vide Haryana Act 26 of 2014

**PROGRAMME BOOKLET**  
**M.Sc. Chemistry (CHP01)**  
**(Batch: 2022-2024)**  
**(Syllabus: Scheme B)**  
**Department of Chemistry**  
**School of Applied Sciences**  
**Manav Rachna University**

# **MANAV RACHNA UNIVERSITY**

## **Vision**

To educate students in frontier areas of knowledge enabling them to take up challenges as ethical and responsible global citizens

## **Mission**

- To impart outcome based holistic education
- To disseminate education in frontier areas
- To produce globally competitive, ethical and socially responsible human resources
- To produce human resources sensitive to issues of Environment and Sustainable Development
- To develop Environment and Sustainable development as a thrust area of research and development.

## **Quality Policy**

To continuously learn from the best practices, study role models and develop transparent procedures for empowerment of stakeholders.

## **Strategic Objectives**

- To facilitate, enhance & promote innovation in curriculum design and delivery and have Outcome-oriented Learning Culture.
- To promote Research Environment and Management Practices.
- To enhance the quality of the student learning experience.
- To provide Resources and Infrastructure for Academic Excellence.

# **DEPARTMENT OF CHEMISTRY**

## **Vision**

To educate students in frontier areas of sustainable chemistry aspects through research and innovation for the society.

## **Mission**

- To impart outcome based holistic education in thrust areas of the chemistry.
- To produce globally competent and socially responsible citizens.
- To develop human resource with better ethical and moral values.
- To innovate environmentally benign products using alternative approaches of the chemistry.

# M.Sc. Chemistry

## Programme Educational Objectives (PEOs)

- **Preparation:** A broad general education assuring an adequate foundation in mathematics, science relevant to computer engineering.
- **Core Competence:** A solid understanding of concepts fundamental to the discipline of computer science engineering.
- **Breadth:** Good analytic, design and implementation skills required to formulate and solve computing problems.
- **Professionalism:** The ability to function and communicate effectively as ethically socially responsible computer science engineering professionals.
- **Learning Environment:** To provide student awareness of the life-long learning and provide a familiarity with professional issues in computer science engineering: ethics, emerging technologies, and fostering of important job related skills.

## Programme Outcomes (POs)

- Graduates will demonstrate knowledge of Chemistry and chemical technologies.
- Graduates will be able to design, carry out, record and analyze the results of chemical experiments.
- Graduates will be able to use modern instrumentation and classical techniques, to design experiments, and to properly record the results of their experiment.
- Graduates will be skilled in problems solving, critical thinking and analytical reasoning.
- Students will have a firm foundation in the fundamentals and application of current chemical and scientific theories including those in Analytical, Inorganic, Organic and Physical Chemistries.
- Graduates will demonstrate skills to use modern chemical equipments to solve an issue related to Chemistry.
- Graduates will demonstrate knowledge to use modern library searching and retrieval methods to obtain information about a topic.
- Graduates will be able to communicate effectively in both verbal and written form.
- Graduates will show the understanding to identify and solve chemical problems and explore new areas of research.
- Graduates will develop confidence for self-education and ability for life-long learning.
- Graduates can participate and succeed in competitive examinations.

**MANAV RACHNA UNIVERSITY FARIDABAD**  
**DEPARTMENT OF CHEMISTRY**  
**MSc Chemistry (CHP01)**  
**SCHEME-B (Effective from July 2022)**

**SEMESTER I**

| Subject Codes                                | Subject Name          | Offering Department | Course Nature (Hard/ Soft/ NTCC) | Course Type (Core/ Elective) | L         | T        | P         | Contact Hours Per Week | No. Of Credits |
|--|-----------------------|---------------------|----------------------------------|------------------------------|-----------|----------|-----------|------------------------|----------------|
| CHH501B                                      | Physical Chemistry-I  | CH                  | Hard                             | Core                         | 4         | 0        | 0         | 4                      | 4              |
| CHH502B                                      | Inorganic Chemistry-I | CH                  | Hard                             | Core                         | 4         | 0        | 0         | 4                      | 4              |
| CHH503B                                      | Organic Chemistry-I   | CH                  | Hard                             | Core                         | 4         | 0        | 0         | 4                      | 4              |
| CHH504B                                      | Analytical Chemistry  | CH                  | Hard                             | Core                         | 4         | 0        | 0         | 4                      | 4              |
| CHH505B                                      | Laboratory-I          | CH                  | Practical                        | Core                         | 0         | 0        | 12        | 12                     | 6              |
| <b>Total (L-T-P-O/Contact Hours/Credits)</b> |                       |                     |                                  |                              | <b>16</b> | <b>0</b> | <b>12</b> | <b>28</b>              | <b>22</b>      |

**SEMESTER II**

| Subject Codes                                | Subject Name            | Offering Department | Course Nature (Hard/Soft/ NTCC) | Course Type (Core/ Elective) | L         | T        | P         | Contact Hours Per Week | No. Of Credits |
|--|-------------------------|---------------------|---------------------------------|------------------------------|-----------|----------|-----------|------------------------|----------------|
| CHH506B                                      | Physical Chemistry-II   | CH                  | Hard                            | Core                         | 4         | 0        | 0         | 4                      | 4              |
| CHH507B                                      | Inorganic Chemistry-II  | CH                  | Hard                            | Core                         | 4         | 0        | 0         | 4                      | 4              |
| CHH508B                                      | Organic Chemistry-II    | CH                  | Hard                            | Core                         | 4         | 0        | 0         | 4                      | 4              |
| CHH509B                                      | Molecular Spectroscopy  | CH                  | Hard                            | Core                         | 4         | 0        | 0         | 4                      | 4              |
| CHH510B                                      | Laboratory-II           | CH                  | Practical                       | Core                         | 0         | 0        | 8         | 8                      | 4              |
| CHS620                                       | Computational Chemistry | CH                  | Soft                            | Domain Elective              | 1         | 0        | 2         | 3                      | 2              |
| RDO503                                       | Scientific Research-I   | CH                  | NTCC                            | Core                         | 0         | 0        | 8         | 2                      | 4              |
| <b>Total (L-T-P-O/Contact Hours/Credits)</b> |                         |                     |                                 |                              | <b>17</b> | <b>0</b> | <b>18</b> | <b>29</b>              | <b>26</b>      |

## Physical Chemistry Specialization

### SEMESTER III

| Subject Codes                         | Subject Name  | Offering Deptt. | Course Nature (Hard/Soft / NTCC) | Course Type (Core/Elective) | L  | T | P  | Contact Hours Per Week | No. Of Credits |
|---------------------------------------|---|-----------------|----------------------------------|-----------------------------|----|---|----|------------------------|----------------|
| CHH601B                               | Symmetry & Group Theory   | CH              | Hard                             | Core                        | 4  | 0 | 0  | 4                      | 4              |
| CHH602B                               | Physical Special-I (Magneto-chemistry, Chemical Kinetics, Catalysis & ion transport)                    | CH              | Hard                             | Special Core                | 4  | 0 | 0  | 4                      | 4              |
| CHH603B                               | Physical Special-II (Irreversible thermodynamics, Transport Phenomenon, Photochemistry & Fast Reaction) | CH              | Hard                             | Special Core                | 4  | 0 | 0  | 4                      | 4              |
| CHH604B /CHH605 B                     | Physical Elective: (Advanced Spectroscopy/ Advanced Chemical Kinetics)                                  | CH              | Hard                             | Special Core                | 4  | 0 | 0  | 4                      | 4              |
| CHH606B                               | Physical Laboratory   | CH              | Practical                        | Core                        | 0  | 0 | 8  | 8                      | 4              |
| RDO603                                | Scientific Research-II  | CH              | NTCC                             | Core                        | 0  | 0 | 8  | 2                      | 4              |
| Total (L-T-P-O/Contact Hours/Credits) |   |                 |                                  |                             | 16 | 0 | 16 | 26                     | 24             |

## Inorganic Chemistry Specialization

### SEMESTER III

| Subject Codes                                | Subject Name  | Offering Deptt | Course Nature (Hard/Soft /Ntcc) | Course Type (Core/ Elective) | L         | T        | P         | Contact Hours Per Week | No. Of Credits |
|--|---|----------------|---------------------------------|------------------------------|-----------|----------|-----------|------------------------|----------------|
| CHH601B                                      | Symmetry & Group Theory   | CH             | Hard                            | Core                         | 4         | 0        | 0         | 4                      | 4              |
| CHH608B                                      | Inorganic Special-I (Organometallic Chemistry of Transition Metals & Bio Inorganic Chemistry) | CH             | Hard                            | Special Core                 | 4         | 0        | 0         | 4                      | 4              |
| CHH609B                                      | Inorganic Special-II (Supramolecular Chemistry & Metal Clusters)                              | CH             | Hard                            | Special Core                 | 4         | 0        | 0         | 4                      | 4              |
| CHH610B /CHH611 B                            | Inorganic Elective (Solid state Materials / Inorganic & Biological Catalysis)                 | CH             | Hard                            | Special Core                 | 4         | 0        | 0         | 4                      | 4              |
| CHH612B                                      | Inorganic Laboratory  | CH             | Practical                       | Core                         | 0         | 0        | 8         | 8                      | 4              |
| RDO603                                       | Scientific Research-II  | CH             | NTCC                            | Core                         | 0         | 0        | 8         | 2                      | 4              |
| <b>Total (L-T-P-O/Contact Hours/Credits)</b> |   |                |                                 |                              | <b>16</b> | <b>0</b> | <b>16</b> | <b>26</b>              | <b>24</b>      |

**Organic Chemistry Specialization**  
**SEMESTER III**

| Subject Codes                   | Subject Name  | Offering Deptt | Course Nature (Hard/Soft /NTCC) | Course Type (Core/ Elective) | L         | T        | P         | Contact Hours Per Week | No. Of Credits |
|---------------------------------|---|----------------|---------------------------------|------------------------------|-----------|----------|-----------|------------------------|----------------|
| CHH601B                         | Symmetry & Group Theory   | CH             | Hard                            | Core                         | 4         | 0        | 0         | 4                      | 4              |
| CHH613B                         | Organic Special-I<br>(Statistical Stereochemistry & Asymmetric Synthesis)   | CH             | Hard                            | Special Core                 | 4         | 0        | 0         | 4                      | 4              |
| CHH614B                         | Organic Special-II<br>(Photochemistry & Pericyclic Reaction)  | CH             | Hard                            | Special Core                 | 4         | 0        | 0         | 4                      | 4              |
| CHH615B/<br>CHH616B/<br>CHH617B | Organic Elective<br>(Modern Organic Synthetic Technique /<br>Bioorganic Chemistry/<br><br>Chemistry of Natural Products | CH             | Hard                            | Special Core                 | 4         | 0        | 0         | 4                      | 4              |
| CHH618B                         | Organic Laboratory  | CH             | Practical                       | Core                         | 0         | 0        | 8         | 8                      | 4              |
| RDO603                          | Scientific Research-II  | CH             | NTCC                            | Core                         | 0         | 0        | 8         | 2                      | 4              |
|                                 | <b>Total (L-T-P-O/Contact Hours/Credits)</b>  |                |                                 |                              | <b>16</b> | <b>0</b> | <b>16</b> | <b>26</b>              | <b>24</b>      |



**SEMESTER IV**  
**(Common for All Specializations)**

| Subject Codes                                | Subject Name  | Offering Department | *Course Nature (Hard/Soft/NTCC) | Course Type (Core/Elective Etc) | L        | T        | P        | O         | Contact Hours Per Week | No. Of Credits |
|--|---|---------------------|---------------------------------|---------------------------------|----------|----------|----------|-----------|------------------------|----------------|
| CHN619B                                      | Major Project (Industrial or Research Lab Training) | CH                  | NTCC                            | Core                            | 0        | 0        | 0        | 12        | 0                      | 12             |
| <b>Total (L-T-P-O/Contact Hours/Credits)</b> |   |                     |                                 |                                 | <b>0</b> | <b>0</b> | <b>0</b> | <b>12</b> | <b>0</b>               | <b>12</b>      |

**TOTAL CREDITS FOR SEMESTER I –IV**

| S.No.  | Semester        | Classroom Contact Hours | Non Teaching Outcome Hrs | Credits   |
|--|-----------------|-------------------------|--------------------------|-----------|
| 1  | First Semester  | 28                      | 0                        | 22        |
| 2  | Second Semester | 29                      | 0                        | 26        |
| 3  | Third Semester  | 26                      | 0                        | 24        |
| 4  | Fourth Semester | 0                       | 12                       | 12        |
| <b>Total Credits For M.Sc. Chemistry Programme</b> |                 | <b>83</b>               | <b>0</b>                 | <b>84</b> |

**SECTION WEIGHTAGE PARAMETERS**

| Syllabus | Sections     | Weightage   |
|----------|--------------|-------------|
|          | A            | 25%         |
|          | B            | 25%         |
|          | C            | 25%         |
|          | D            | 25%         |
|          | <b>TOTAL</b> | <b>100%</b> |

# SEMESTER I

|                          |  |
|--------------------------|--|
| <b>Course Title/Code</b> | <b>Physical Chemistry-I (CHH501B)</b>  |
| <b>Course Type</b>       | Core   |
| <b>Course Nature</b>     | Hard   |
| <b>L-T-P-O Structure</b> | 4-0-0-0  |
| <b>Objectives</b>        | To impart knowledge of electrochemistry and kinetics of chemical reactions.<br>To impart knowledge of surface chemistry and catalysis  |
| <b>Outcome</b>           | Students will be able to understand concepts of electrochemistry and kinetics of chemical reactions<br>Students will be able to understand the role of catalyst on its absorption behavior |
| <b>Prerequisites</b>     | B.Sc. with Chemistry as one of the Subject   |

#### SECTION-A

**Electrochemistry:** Solutions: Activity coefficients and ion-ion interactions. Physical significance of activity coefficients, mean activity coefficient of an electrolyte and its determination, Derivation of the Debye-Hückel theory of activity coefficients (both point ion size and finite ion size models), Excess functions, Metal/Electrolyte interface: Introduction and characteristics (OHP and IHP, potential profile across double layer region)

#### SECTION-B

**Surface phenomena:** Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micelle concentration (CMC), Krafft temperature, Factors affecting the CMC of surfactants, counterion binding to micelles, thermodynamics of micellization, solubilization, microemulsions, reverse micelles, surface films (electrokinetic phenomena), catalytic activity at surfaces. Electrode/ electrolyte interface; Nernst equation.

#### SECTION-C

**Quantum Chemistry:** Postulates of Quantum mechanics, Linear and Hermitian operators, Turn-over rule, Commutation of operators and Uncertainty principle. Some exactly soluble problems: Particle in a box (1-D, 2-D & 3-D) and ring. Concept of degeneracy and its application to Jahn-Teller distortion, Simple harmonic oscillator problem and its solution using series solution or factorization method, Calculation of various average values, Brief Description: Angular momentum operators, Eigen values and eigen-functions, Radial distributions.

#### SECTION-D

**Approximate methods:** First order time-independent perturbation theory for non-degenerate states, Variation theorem and variational methods, Use of these methods illustrated with some examples (particle in a box with a finite barrier, anharmonic oscillator, and approximate functions for particle in a box and hydrogen atom).

**HMO method and its applications:**  $\pi$ -Electron approximation, Huckel Molecular Orbital Theory of conjugated systems Ladder operators and recursion relations of Hermite polynomials, Generating functions, Rodrigues Representation. Derivation of rigid rotator and H-atom (energy quantization)

#### Books Recommended

1. J. M. Bockris and A. K. N. Reddy, Modern Electrochemistry 1 (Ionics), Springer (2006).

2. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
3. Lowe, J. P. & Peterson, K. *Quantum Chemistry* Academic Press (2005).
2. McQuarrie, D. A. *Quantum Chemistry* Viva Books Pvt Ltd.: New Delhi (2003).
3. Mortimer, R. G. *Mathematics for Physical Chemistry* 2nd Ed. Elsevier (2005).
4. Pilar F. L. *Elementary Quantum Chemistry* 2nd Ed., Dover Publication Inc.: N.Y. (2001).
5. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
6. Levine, I. L. *Quantum Chemistry* 5th Ed., Prentice-Hall Inc.: New Jersey (2000).

|                          |   |
|--------------------------|---|
| <b>Course Title/Code</b> | <b>Inorganic Chemistry-I (CHH502B)</b>  |
| <b>Course Type</b>       | Core  |
| <b>Course Nature</b>     | Hard  |
| <b>L-T-P-O Structure</b> | 4-0-0-0   |
| <b>Objectives</b>        | To familiarize students with Metal-Ligand Bonding in Transition Metal Complexes<br>To impart knowledge on Electronic Spectra of Transition Metal Complexes  |
| <b>Outcome</b>           | The students will be able to understand ML bonding in transition metal complexes.<br>The students will be able to understand electronic spectra of transition metal complexes.<br>The students will be able to understand VSEPR and HSAB theory |
| <b>Prerequisites</b>     | B.Sc. with Chemistry as one of the Subject  |

#### SECTION-A

**Metal-Ligand Bonding In Transition Metal Complexes:** Crystal field theory, CFT splitting of d orbitals in octahedral, tetrahedral and square planar complexes, factors affecting CFT, CFSE, applications of CFT, Spectrochemical series and effects of covalency. Nephelauxetic series, magnetic properties of transition metal complexes, Jahn-Teller distortions, Jahn Teller stabilization energy; molecular orbital theory of octahedral complexes

#### SECTION-B

**Electronic Spectra Of Transition Metal Complexes:** Types of transition, selection rules for electronic transitions and relaxation of selection rules, width of absorption bands, electronic spectra of transition metal complexes, Term-symbols, Russel-Saunders states, Spectroscopic ground states; Coupling schemes, Orgel diagrams, determination of  $Dq$  and Racah parameters, Charge transfer spectra (MLCT, LMCT).

#### SECTION-C

**Organometallic Chemistry-I:** Classification of organometallic compounds, nomenclature, EAN, 18 e rule, reactions: oxidative addition, reductive elimination, insertion;  $\sigma$  bonded organometallic

compounds and  $\Pi$  bonded organometallic compounds, role of organometallic compounds in catalysis (hydrogenation, hydroformylation)

#### SECTION-D

**Metal Carbonyls:** Classification of metal carbonyls (mono, bi, poly, bridging), general method of preparation, structure of metal carbonyl, vibrational spectra of metal carbonyls for bonding and structural elucidation (homoleptic and heteroleptic), introduction to tertiary phosphine as ligands.

#### Books Recommended

1. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles of Structure and Reactivity, 4<sup>th</sup> ed. Pearson Education, 2006.
2. P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver & Atkins: Inorganic Chemistry, 4<sup>th</sup> ed. Oxford University Press, 2006.
3. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6<sup>th</sup> ed. Wiley, 1999.
4. R. C. Mehrotra and A. Singh, Organometallic Chemistry: A Unified Approach, New Age International, 2006.
5. A. J. Elias, B. D. Gupta; Basic Organometallic Chemistry: Concepts, Synthesis and Applications of Transition metals, CRC Press and Universities Press, 2010.
6. J. D. Lee; Concise Inorganic Chemistry, 4<sup>th</sup> ed. Chapman and Hall, 1991

|                          |   |
|--------------------------|---|
| <b>Course Title</b>      | <b>Organic Chemistry-I (CHH 503B)</b>   |
| <b>Course Type</b>       | Core  |
| <b>Course Nature</b>     | Hard  |
| <b>L-T-P-O Structure</b> | 4-0-0-0   |
| <b>Objectives</b>        | To familiarize with reactive intermediates of organic chemistry and its generation.<br>To impart knowledge of Nucleophilic Substitution and reactivity effects of substrate structure<br>To impart knowledge of nucleophilic and electrophilic aromatic substitution reactions<br>To impart the knowledge of neighboring groups effect on product formation |
| <b>Outcome</b>           | Students will be able to understand the concept of reactive intermediate in organic chemistry.<br>Students will be able to grasp in depth knowledge of Nucleophilic and Electrophilic Substitution reactions and its implications on various organic reactions<br>Students will be able to understand the neighboring group effect on product formation     |
| <b>Prerequisites</b>     | B.Sc. with Chemistry as one of the Subject  |

#### SECTION A

#### Reactive Intermediates in Organic Chemistry

**Carbocations:** Classical and non-classical, neighbouring group participation, ion-pairs, molecular rearrangements in acyclic, monocyclic and bicyclic systems, stability and reactivity of bridge-head carbocations.

**Carbanions:** Generation, structure and stability, ambident ions and their general reactions; HSAB principle and its applications.

**Free Radicals:** Generation, structure, stability and reactions, cage effects; radical-cations & radical anions,

**Carbenes:** Formation and structure, reactions involving carbenes and carbenoids.

**Nitrenes:** Generation, structure and reactions of nitrenes.

**Arynes:** Generation and reactivity of arynes, nucleophilic aromatic substitution reactions, S<sub>N</sub>Ar mechanism; Ipso effect.

## SECTION B

**Nucleophilic Substitution at Saturated Carbon:** Mechanism and Stereochemistry of S<sub>N</sub>1 and S<sub>N</sub>2, S<sub>N</sub>i reactions. The reactivity effects of substrate structure, solvent effects, competition between S<sub>N</sub>1 and S<sub>N</sub>2 mechanisms

## SECTION-C

**ELECTROPHILIC AROMATIC SUBSTITUTION:** The Arenium ion mechanism, orientation and reactivity in monosubstituted benzene rings, ortho/ para ratio. Ipso substitution

**NUCLEOPHILIC AROMATIC SUBSTITUTION:** The Aromatic S<sub>N</sub>1, S<sub>N</sub>2 and benzyne mechanisms. Reactivity – effect of substrate structure, leaving group, and attacking nucleophilic

## SECTION-D

**Neighbouring Group Participation:** Evidences of N.G.P.; the phenonium ion, participation by π and σ bonds, Anchimeric assistance, Classical versus non-classical carbonium ions

### Books recommended

1. M.B. Smith and J. March; March's Advanced Organic Chemistry, 5<sup>th</sup> Edition, John Wiley & Sons, New York, 2001
2. P. Sykes; A Guide book to Mechanism in Organic Chemistry, 6<sup>th</sup> Edition, Orient Longman Ltd., New Delhi, 1997
3. S. M. Mukherjee and S.P. Singh; Reaction Mechanism in Organic Chemistry, 1<sup>st</sup> ed. Macmillan India Ltd., New Delhi, 1990
4. I. L. Finar; Organic Chemistry, Vol. II, 5th Edition, ELBS and Longman Ltd, New Delhi, 1996
5. R.T. Morrison and R.N. Boyd; Prentice: Organic Chemistry, 6th Edition, 1992.

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|--------------------------|--|
| <b>Course Title/Code</b> | <b>ANALYTICAL CHEMISTRY (CHH 504B)</b>   |
| <b>Course Type</b>       | Core   |
| <b>Course Nature</b>     | Hard   |
| <b>L-T-P-O Structure</b> | 4-0-0-0  |
| <b>Objectives</b>        | To impart knowledge on various analytical techniques<br>To familiarize with the principle of analytical chemometrics   |
| <b>Outcome</b>           | Students will be able to Understand various analytical techniques<br>Students will be able to understand factor analysis, resolution and pattern recognition |
| <b>Prerequisites</b>     | B.Sc. with Chemistry as one of the Subject   |

## SECTION A

**Analytical chemistry** and chemical analysis, Classification of analytical methods, Method selection, Sample processing, Steps in a quantitative analysis, Data organization, analytical validations, Limit of detection and limit of quantization.

**Atomic Spectroscopy:** Atomic absorption (AAS), emission (AES) and inductively coupled plasma (ICP) spectroscopy.

## SECTION B

**Photoelectron Spectroscopy:** Principle and Instrumentation, Types of Photoelectron Spectroscopy – UPS & XPS Binding Energies, Koopman's Theorem, Chemical Shifts. Photoelectron Spectra of Simple Molecules: N<sub>2</sub>, O<sub>2</sub>, F<sub>2</sub>, CO, HF, NH<sub>3</sub> and H<sub>2</sub>O - ESCA in qualitative analysis, Principles of Auger electron spectroscopy.

## SECTION C

**Optical Methods:** Electronic spin resonance spectra, Mossbauer spectroscopy.

Theory, Instrumentation and applications of X-rays (emission, absorption, diffraction Methods)

Capillary electrophoresis, Potentiometry, Coulometry, Voltametry

## SECTION D

**Chromatographic Techniques:** HPLC, HPTLC and GC its instrumentation, working, applications and limitations, Supercritical Chromatography.

**Imaging Techniques** – Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM)

**Hyphenated Techniques:** HPLC-MS, GC-MS, GC-IR, ICP-MS and TLC-MS

### Books Recommended

1. D. A. Skoog; Principles of Instrumental Analysis, 5<sup>th</sup> ed. Saunders College Publishing, Philadelphia, London, 1998
2. G.W. Ewing; Instrumental Methods of Chemical Analysis, 5<sup>th</sup> ed. McGraw Hill Books Co., New York, 1978
3. J.H. Kennedy, Analytical Chemistry: Principles, 2<sup>nd</sup> ed. Saunders Holt, London, 1990
4. G. D. Christian; Analytical Chemistry, 5<sup>th</sup> ed. John Wiley & Sons, New York, 1994
5. R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William; Modern Methods of Chemical Analysis, 2<sup>nd</sup> ed. John Wiley, New York, 1976
6. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch; Analytical Chemistry - An Introduction, 7<sup>th</sup> ed. Saunders College Publishing, Philadelphia, London, 2000

|                          |  |
|--------------------------|--|
| <b>Course Title/Code</b> | <b>LABORATORY WORK-I (CHH 505B)</b>  |
| <b>Course Type</b>       | Core   |
| <b>Course Nature</b>     | Hard   |
| <b>L-T-P-O Structure</b> | 0-0-12-0   |
| <b>Objectives</b>        | To Familiarize students with gravimetric and volumetric analysis of inorganic compounds<br>To Familiarize students with identification of organic compounds having one or more functional groups |

|                      |  |
|----------------------|--|
| <b>Outcome</b>       | The students will be able to do gravimetric and volumetric analysis of inorganic compounds<br>The students will be able to understand qualitative analysis of mixture containing five cation |
| <b>Prerequisites</b> | B.Sc. with Chemistry as one of the Subject   |

### LIST OF EXPERIMENTS

1. To prepare crystals of tetra-amine copper (II) sulphate  $[\text{Cu}(\text{NH}_3)_4] \text{SO}_4$ .
2. To prepare Nickel Dimethylglyoxime Complex  $[\text{Ni}(\text{DMG})_2]$  using Dimethylglyoxime
3. To prepare crystals of Sodium Ferrioxalate  $\text{Na}_3[\text{Fe}(\text{C}_2\text{O}_4)_3] \cdot 9\text{H}_2\text{O}$
4. To estimate magnesium in standard  $\text{MgSO}_4$  solution using M/100 EDTA in complexometric titration using Eriochrome Black T indicator titrimetrically
5. To estimate amount of calcium in standard  $\text{CaCO}_3$  solution using M/10 EDTA in complexometric titration using Eriochrome Black T indicator titrimetrically
6. To prepare crystals of Chrome Alum  $[\text{K}_2\text{SO}_4\text{Cr}_2(\text{SO}_4)_3 \cdot 24\text{H}_2\text{O}]$
7. To estimate Aluminium or aluminium oxide in potash alum or ammonium aluminium sulphate.
8. To estimate  $\text{Ni}^{2+}$  gravimetrically as Nickel dimethyl glyoxime (Ni-DMG) complex using DMG
9. To estimate  $\text{Ba}^{2+}$  gravimetrically as barium chloride

### Books Recommended

1. A. Gaddamwar and P. R. Rajput, Organic and Inorganic Practical Chemistry, PragatiPrakashan, 2010
2. R. W. Helmkamp; A Text-book of Practical Organic Chemistry Including Qualitative Organic Analysis, Longman Green and Co. New York, 1956
3. J. Singh and L. D. S. Yadav; Advanced Practical Chemistry, PragatiPrakashan, 2012
4. A. Gaddamwar and P. R. Rajput, Organic and Inorganic Practical Chemistry, PragatiPrakashan, 2010
5. J. Singh and L. D. S. Yadav; Advanced Practical Chemistry, Pragati Prakashan, 2012



# SEMESTER II

|                          |  |
|--------------------------|--|
| <b>Course Title/Code</b> | <b>Physical Chemistry-II (CHH 506B)</b>  |
| <b>Course Type</b>       | Core   |
| <b>Course Nature</b>     | Hard   |
| <b>L-T-P-O Structure</b> | 4-0-0-0  |
| <b>Objectives</b>        | To familiarize with concept of Quantum Chemistry in statistical thermodynamics<br>To impart knowledge of Statistical Thermodynamics  |
| <b>Outcome</b>           | Students will be able to understand corrosion cause and type<br>Students will be able to understand Statistical Thermodynamics in relation to the Concepts of distribution and thermodynamic probability |
| <b>Prerequisites</b>     | Physical Chemistry-I   |

#### SECTION-A

**Statistical Mechanics:** Fundamentals: Idea of microstates and macrostates, Concept of distributions- Binomial & multi-nomial distributions for non-degenerate and degenerate systems, Thermodynamic probability and most probable distribution, Canonical and other ensembles, Statistical mechanics for systems of independent particles and its importance in chemistry, Types of statistics: Boltzmann, Bose-Einstein and Fermi-Dirac statistics, Thermodynamic probability (W) for the three types of statistics, Derivation of distribution laws (most probable distribution) for the three types of statistics, Lagrange's undetermined multipliers, Stirling's approximation, Molecular partition function and its importance, Assembly partition function

#### SECTION-B

**Thermodynamics Applications to ideal gases:** The molecular partition function and its factorization, Evaluation of translational, rotational and vibrational partition functions for monatomic, diatomic and polyatomic gases, The electronic and nuclear partition functions, Calculation of thermodynamic properties of ideal gases in terms of partition function, Statistical definition of entropy, Ortho- and para-hydrogen, statistical weights of ortho and para states, symmetry number, Calculation of equilibrium constants of gaseous solutions in terms of partition function, perfect gas mixtures.

#### SECTION-C

**Diffraction Methods:** Atomic scattering factors, Scattering by a small crystal, Direct and reciprocal lattice, Miller indices, Bragg's law and Laue's equations, Structure factor, Systematic absences for different types of unit cells (primitive, face-centred, body-centred, side-centred) and application to some common metal and metal salt structures (rock salt, zinc blende). Space groups, Glide planes

and screw axes, Structure determination for organic crystals like naphthalene, Fourier series **Patterson's functions** Heavy atom method, Comparison of X-ray method with electron and neutron diffraction methods,

#### SECTION-D

**Kinetics:** *Theories of reaction rates:* Collision theory, Potential energy surfaces (basic idea), Transition state theory (both thermodynamic and statistical mechanics formulations), Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment, RRKM model (qualitative treatment)

**Solution kinetics:** Factors affecting reaction rates in solution, Effect of solvent and ionic Strength (primary salt effect) on the rate constant, Secondary salt effects

#### Books Recommended

1. McQuarrie, D. A. *Statistical Mechanics* Viva Books Pvt. Ltd.: New Delhi (2003).
2. Bagchi B. *Statistical Mechanics for Chemistry and Material Science*, CRC Press (2018).
3. L. D. Landau and E. M. Lifshitz, *Statistical Mechanics, Part I*, Butterworth-Heinemann, 3rd ed. (2005).
4. Kakkar, R., *Atomic & Molecular Spectroscopy* Cambridge University Press (2015).
5. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
6. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).

|                          |  |
|--------------------------|--|
| <b>Course Title/Code</b> | <b>Inorganic Chemistry-II (CHH 507B)</b>   |
| <b>Course Type</b>       | Core   |
| <b>Course Nature</b>     | Hard   |
| <b>L-T-P-O Structure</b> | 4-0-0-0  |
| <b>Objectives</b>        | To familiarize with kinetics of substitution reactions<br>To impart knowledge on electron transfer reactions   |
| <b>Outcome</b>           | The students will be able to understand Kinetics and Mechanism of Substitution Reactions<br>The students will be able to understand electron transfer reaction |
| <b>Prerequisites</b>     | Inorganic Chemistry-I  |

#### SECTION-A

**Kinetics And Mechanism Of Substitution Reactions-I:** Mechanisms of substitution reactions of tetrahedral, square planar, trigonal bipyramidal, square pyramidal and octahedral complexes; Potential energy diagrams, transition states and intermediates, Substitution reactions in octahedral complexes their mechanisms and kinetics, concept of lability and inertness on the basis of VBT and CFT, rate laws (Eigen-Wilkins mechanism, Fuoss Eigen equation), Acid hydrolysis, Base hydrolysis.

#### SECTION-B

**Kinetics And Mechanism Of Substitution Reactions-II:** Substitution in Square Planar Complexes, kinetics, Berry pseudorotation, Trans Effect and its applications to synthesis of

complexes, theories of trans effect, mechanism, factors affecting rate of substitution, applications of complexes.

Metal complex sensitizers: Electron relay, semiconductor supported metal oxide systems, water photolysis, nitrogen fixation and CO<sub>2</sub> reduction.

### SECTION-C

**Electron Transfer Reactions-I** : Mechanism and rate laws; various types of electron transfer reactions (outer and inner sphere), HOMO and LUMO of oxidant and reductant, chemical activation. Precursor complex formation and rearrangement, Marcus-Husch theory, Nature of bridge ligands, fission of successor complexes, Two-electron transfers, Synthesis of coordination compounds using electron transfer reactions, mixed valence complexes and internal electron transfer.

### SECTION-D

**Electron Transfer Reactions-II**: Redox reactions of metal complexes in excited states, correlation between thermal and optical electron transfer reactions; excited electron transfer reactions using [Ru(bpy)<sub>3</sub>]<sup>2+</sup> complex and [Fe(bpy)<sub>3</sub>]<sup>3+</sup> complex as examples. Role of spin-orbit coupling, life-times of excited states in these complexes

### Books Recommended

1. F. Basalo and R. G. Pearson; Mechanism of Inorganic Reactions, 2<sup>nd</sup> ed. Wiley Eastern Ltd., New Delhi, 1967
2. D. F. Shriver and P. W. Atkins; Inorganic Chemistry, 3<sup>rd</sup> ed. ELBS, London, 1999
3. F. A. Cotton and G. Wilkinson; Advanced Inorganic Chemistry, 6<sup>th</sup> ed. John Wiley & Sons, New York, 1999
4. D.N. Sathyanarayana; Electronic Absorption Spectroscopy and Related Technique, Universities Press (India) Ltd., Hyderabad, 2001
5. K.F. Purcell, J.C. Kotz; Inorganic chemistry, Saunders, 1977

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| <b>Course Title/Code</b> | <b>Organic Chemistry-II (CHH 508B)</b>  |
| <b>Course Type</b>       | Core  |
| <b>Course Nature</b>     | Hard  |
| <b>L-T-P-O Structure</b> | 4-0-0-0   |
| <b>Objectives</b>        | To familiarize carbon carbon multiple bond, aromaticity linear free energy relationship and advance heterocyclic reactions<br>To impart knowledge on Elimination reactions  |
| <b>Outcome</b>           | Able to understand carbon carbon multiple bond, aromaticity linear free energy relationship and advance heterocyclic reactions<br>Able to understand about Elimination reactions and its implication in organic chemistry |
| <b>Prerequisites</b>     | Organic Chemistry-I   |

### SECTION A

**Addition To Carbon–Carbon Multiple Bonds**: Electrophilic, free-radical and nucleophilic addition: Mechanistic and Stereo chemical aspects involving electrophiles, nucleophiles and free radicals, regio– and chemoselectivity, Orientation and reactivity. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration and Michael reaction, Sharpless Epoxidation.

## SECTION B

**Elimination Reactions:** The E1, E2 and E1Cb (Elimination Unimolecular conjugate Base) mechanisms, Orientation of the double bond. Hofmann versus Saytzeff elimination, Pyrolytic syn-elimination, Competition between substitution and elimination reactions

## SECTION C

**Nature of Bonding in Organic molecules:** Delocalized chemical bonding –conjugation, cross conjugation, resonance, hyperconjugation, tautomerism. Aromaticity in benzenoid and nonbenzenoid compounds, alternante and non-alternante hydrocarbons, Huckel's rule

**Effects Of Structure On Reactivity:** Linear free energy relationships (LFER), the Hammett equation – substituent and reaction constants; the Taft treatment of polar and steric effects in aliphatic compounds

## SECTION D

**Heterocyclics With Two Hetero Atoms:** Synthesis, reactivity, aromatic character and importance of the following heterocycles: Indole, Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine, Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

### Books recommended

1. M.B. Smith and Jerry March; March's Advanced Organic Chemistry, 5<sup>th</sup>ed. John Wiley & Sons, New York, 2001
1. P. Sykes; A Guide Book to Mechanism in Organic Chemistry, 6<sup>th</sup> ed. Orient Longman Ltd., New Delhi, 1997
2. S. M. Mukherjee and S.P. Singh; Reaction Mechanism in Organic Chemistry, 1<sup>st</sup>ed. Macmillan India Ltd., New Delhi, 1990
3. T.H. Lowry and K. S. Richardson; Mechanism and Theory in Organic Chemistry, 3<sup>rd</sup>ed. Addison – Wesley Longman Inc., 1998
4. P. S. Kalsi; Organic Reactions and Their Mechanisms, 1<sup>st</sup>ed. New Age International Pub., New Delhi, 1996

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| <b>Course Title/Code</b> | <b>MOLECULAR SPECTROSCOPY (CHH 509B)</b>   |
| <b>Course Type</b>       | Core   |
| <b>Course Nature</b>     | Hard   |
| <b>L-T-P-O Structure</b> | 4-0-0-0  |
| <b>Objectives</b>        | To familiarize with PMR and CMR<br>To impart knowledge on mass spectroscopy for studying the fragmentation pattern   |
| <b>Outcome</b>           | Students will be able to understand principle of PMR, CMR and ESR spectroscopy<br>Students will be able to understand Photoelectron Spectroscopy<br>Students will be able to analysis fragmentation pattern of the compound by mass spectrometry |
| <b>Prerequisites</b>     | Analytical Chemistry   |

## SECTION A

**Spectroscopy-I:** Principle, Instrumentation and application of UV-visible, Molecular luminescence (fluorescence, chemiluminescence, phosphorescence)

Vibrational Spectroscopy: IR spectroscopy (Far IR and near IR), Raman Spectroscopy, Difference between Raman and IR spectra, Emission spectra

### SECTION B

**Spectroscopy-II: PMR:** Natural abundance of  $^{13}\text{C}$ ,  $^{19}\text{F}$  and  $^{31}\text{P}$  nuclei, the spinning nucleus, effect of external magnetic field, precessional motion and frequency Energy transitions Chemical shift and its measurements, factors influencing chemical shift, anisotropic effect, integral of protons spin spin coupling splitting theory magnitude of coupling constant simple, virtual and complex spin coupling, Chemical and magnetic equivalence proton exchange, factors affecting the coupling- First and non first order spectra, simplification of complex spectra (solvent effect, double resonance and field effect).

### SECTION C

**Spectroscopy-III: CMR:** Resolution and multiplicity of  $^{13}\text{C}$  NMR,  $^1\text{H}$ -decoupling noise decoupling, broad band decoupling, Deuterium, fluorine and phosphorus coupling, NOE signal enhancement off-resonance, proton decoupling, structural application of CMR DEPT and INEPT experiments, Introduction to 2D NMR.

### SECTION D

**Spectroscopy-IV: Mass:** Theory, instrumentation and modification Unit mass and molecular ions Important terms single, double/multiple charged ion metastable peak base peak isotopic mass peak, relative intensity etc.

#### Books Recommended-

1. R.M. Silverstein, D. J. Kiemle and F.X. Webster; Spectroscopic identification of organic compounds, 7<sup>th</sup> ed. John Wiley & sons, 2005
2. William Kemp; Organic spectroscopy 3<sup>rd</sup> ed. Palgrave publishing house, 2008
3. M. Rose and R.A. W. Johnstone; Mass Spectrometry for Chemists and biochemists, 2<sup>nd</sup> ed. Cambridge University Press, 2012
4. D.H. Williams and I. Fleming; Spectroscopic methods in organic chemistry, 6<sup>th</sup> ed. McGraw Hill Publishing Co. 1989

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| <b>Course Title/Code</b> | <b>LABORATORY WORK-II (CHH-510-B)</b>   |
| <b>Course Type</b>       | Core  |
| <b>Course Nature</b>     | Hard  |
| <b>L-T-P-O Structure</b> | 0-0-8-0   |
| <b>Objectives</b>        | To familiarize students with Quantitative separation and determination of metal ions        |
| <b>Outcome</b>           | Students will be able to understand Quantitative separation and determination of metal ions |
| <b>Prerequisites</b>     | Laboratory work-I   |

#### INORGANIC CHEMISTRY PRACTICALS

1. Quantitative separation and determination of the following pairs of metal ions using gravimetric and volumetric methods. For example:  $\text{Ag}^+$  (gravimetrically) and  $\text{Cu}^{2+}$  (volumetrically),  $\text{Cu}^{2+}$

(gravimetrically) and  $Zn^{2+}$  (volumetrically),  $Fe^{3+}$ (gravimetrically) and  $Ca^{2+}$  (volumetrically),  $Mg^{2+}$  (gravimetrically) and  $Ca^{2+}$  (volumetrically) etc.

#### ORGANIC CHEMISTRY PRACTICALS

1. Preparation of compounds involving not more than two steps.
2. Identification of organic compounds in given mixture.

#### PHYSICAL CHEMISTRY PRACTICALS

1. Rate constant of acid catalyzed hydrolysis of sucrose by polarimetric method.
2. Rate constant of acid catalyzed hydrolysis of sucrose by chemical method.
3. Rate constant of  $FeCl_3$ -catalyzed  $H_2O$  decomposition by gasometric method.
4. Degree of hydrolysis of urea hydrochloride by kinetics method.

#### Books recommended:

1. A. Gaddamwar and P. R. Rajput; Organic and Inorganic Practical Chemistry, PragatiPrakashan, 2010
2. R. W. Helmkamp; A Text-book of Practical Organic Chemistry Including Qualitative Organic Analysis, Longman Green and Co. New York, 1956
3. J. Singh and L. D. S. Yadav; Advanced Practical Chemistry, PragatiPrakashan, 2012

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| <b>Course Title/Course Code</b> | <b>COMPUTATIONAL CHEMISTRY<br/>(CHS620B)</b>  |
| <b>Course Type</b>              | Domain Elective   |
| <b>Course Nature</b>            | Soft  |
| <b>L-T-P-O structure</b>        | 1-0-2-0   |
| <b>Objectives</b>               | To provide students understanding to use molecular modelling to solve interesting and relevant problems in the core area of chemistry and allied science and technology.  |
| <b>Outcomes</b>                 | Students will be able to <ul style="list-style-type: none"> <li>• CO1: understand principles of Computational Sciences</li> <li>• CO2: compare properties different drugs in computational chemistry in the field of drug discovery</li> <li>• CO3: comprehend relation between the Theoretical and Computational Chemistry</li> <li>• CO4: apply concept of bioinformatics to problem solving</li> </ul> |
| <b>Pre-requisite</b>            |   |

### Section A

#### Introduction to computational Chemistry

Overview and importance of Computational Sciences and its applications to Natural Sciences, Chemistry, Physics, Life Sciences. Modelling process and its types, Computational Toolbox- errors

and their types, rate of change. Importance of Learning Computer Programming in Computational Natural Sciences.

## **Section B**

### **Applications of Computational Sciences in Chemistry**

Computational Quantum Chemistry and its applications, Prediction of Molecular Properties using Computational Chemistry, Overview of Quantum Chemistry Theories and their level of accuracy and hierarchy of computational requirements, Overview of Computer aided drug design and QSAR, Promises of Computational Chemistry

## **Section C**

### **Applications of Computational Chemistry in Life Science**

Introduction to Drugs, classification, Computational resources for drug discovery. Familiarization with Drug data bases tools (Zinc 53, Drug Bank, Chem spider, Chem DB, Med Chem Designer). Smiles of different natural and medicinal compounds. Prediction of Molecular Properties using Computational Chemistry.

## **Section D**

### **Bioinformatics**

Overview of Computational Biology and bioinformatics, Structural Bioinformatics, Genomic data and its interpretation, Molecular Dynamics Simulations on Biological Systems, Hybrid Computational Methods for Studying Structure, Dynamics and Functions of Large Biological Systems, Promises of Computational Biology

### **Hands on Training:**

1. Practical session drug databases tools (Zinc 53, Drug Bank, Chem spider, Chem DB, Med Chem Designer)
2. Solubility prediction of various drug molecule by Swiss ADME
3. Permeability prediction of various drug molecule by Swiss ADME
4. Molecule property prediction by Marvin Sketch
5. Auto docking using simple molecules.

### **Recommended Books and References:**

1. A. B. Shiflet and G. W. Shiflet. Introduction to Computational Sciences (Overseas Press (India) Pvt. Ltd., New Delhi, India), 2011.



2. F. Jensen. Introduction to Computational Chemistry (Second Edition, Wiley), 2007.
3. J. Hasbun, P. Devries. A First Course in Computational Physics. (Viva Books Pvt. Ltd., New Delhi), 2011.
4. D. W. Mount. Bioinformatics (2nd Edition, Cold Spring harbour Press, New Jersey), 2004. 5. Some examples will be taken from Selected Articles from Standard /Reputed Journals.

|                              |   |                          |
|------------------------------|---|--------------------------|
| <b>Course Title/Code</b>     | <b>SCIENTIFIC RESEARCH-I (RDO503)</b>   |                          |
| <b>Course Type</b>           | <b>Core</b>   |                          |
| <b>L-T-P Structure</b>       | <b>0-0-8</b>  |                          |
| <b>Credits</b>               | <b>4</b>  |                          |
| <b>Course Objective</b>      | <b>To impart knowledge on various analytical technique with the principle of analytical chemometrics</b>                          |                          |
| <b>Course Outcomes (COs)</b> |   | <b>Mapping</b>           |
| <b>CO1</b>                   | <b>The student shall be able to describe research and its impact.</b>   | <b>Skill Development</b> |
| <b>CO2</b>                   | <b>The student shall be able to identify broad area of research, analyze, the processes and procedures to carry out research.</b> | <b>Skill Development</b> |
| <b>CO3</b>                   | <b>The student shall be able to use different tools for literature survey</b>   | <b>Skill Development</b> |
| <b>CO4</b>                   | <b>The student is able choose specific area of research and supervisor/mentor is finalized</b>                                    | <b>Skill Development</b> |

|                      |  |                      |
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| <b>CO5</b>           | <b>To understand and adopt the ethical practice that are to be followed in the research activities</b> | <b>Employability</b> |
| <b>CO6</b>           | <b>To work in groups with guidance</b>   | <b>Employability</b> |
| <b>Prerequisites</b> |  |                      |

### **SECTION A**

Unit 1: What is Research and its impact?

**1.1 Capturing the current research trends**

**1.2 Insight about scientific research performed by renowned experts in the related field (case studies)**

**1.3 Do's and Don'ts pertaining to research**

### **SECTION B**

Unit 2: Identification of Broad Area of research

2.1 Identification of thrust area of research for deciding broad area

2.2 Framing the research questions and hypothesis

2.3 Identification of the research gap based on feasibility of problem

2.4 Exploration of in-house and commercially available facilities related to broad area

### **SECTION C**

Unit 3: Understanding the tools for Literature Survey

3.1 Finding research papers related to a topic

3.2 Understanding the different aspects of Literature search

3.3 Usage of different sources like Google scholar, WoS, SCI/ SCIE, PubMed, Scopus, ABDC, EBSCO etc.

3.4 Search for online journals relevant to research area

3.5 Indexing of Journals

3.5 Usage of scholarly networking sites like Research Gate, Mendeley, and Academia.edu etc.

3.6 Demo sessions on the usage of above mentioned sources

### **SECTION D**

Unit 4: Review of research papers pertaining to broad area and specific area of research

4.1 Selection of relevant papers

4.2 Finding specific research problem from broad area of research

4.3 Literature survey and justification of specific research problem

4.4 Experimentation and data cleaning and verification

4.5 Understanding and selection of the research domain

4.6 Seeking information through published work w.r.t the problem

4.7 Reading & categorizing the downloaded/referred papers and structuring of the idea

4.8 Model design about framing the research questions

Unit 5: Report Writing and Presentation skill Development

5.1 Report making on the surveyed literature to cater the basic idea of the research papers

- 5.2 Compiling and analyzing the published results to justify and understand the proposed ideas
- 5.3 Usage of MS-PowerPoint and other technical resources for the presentation
- 5.4 Development of presentation skills and group addressing
- 5.5 Scientific/technical writing and ethical practice, project report

**CO-PO Mapping**

| Course Code   | Course                       | Course Outcomes | PO1      | PO2      | PO3      | PO4      | PO5      | PO6      | PO7      | PO8      | PO9      | PO10     | PO11     |
|---------------|------------------------------|-----------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>RDO503</b> | <b>Scientific Research-I</b> | <b>CO1</b>      | <b>2</b> | <b>2</b> | <b>-</b> | <b>2</b> | <b>2</b> | <b>3</b> | <b>3</b> | <b>3</b> | <b>2</b> | <b>2</b> | <b>2</b> |
|               |                              | <b>CO2</b>      | <b>2</b> | <b>2</b> | <b>-</b> | <b>2</b> | <b>2</b> | <b>2</b> | <b>2</b> | <b>2</b> | <b>2</b> | <b>2</b> | <b>2</b> |
|               |                              | <b>CO3</b>      | <b>-</b> | <b>-</b> | <b>-</b> | <b>-</b> | <b>-</b> | <b>2</b> | <b>3</b> | <b>2</b> | <b>-</b> | <b>-</b> | <b>-</b> |
|               |                              | <b>CO4</b>      | <b>-</b> | <b>-</b> | <b>-</b> | <b>-</b> | <b>-</b> | <b>3</b> | <b>2</b> | <b>2</b> | <b>-</b> | <b>-</b> | <b>-</b> |
|               |                              | <b>CO5</b>      | <b>-</b> | <b>-</b> | <b>-</b> | <b>-</b> | <b>-</b> | <b>2</b> | <b>3</b> | <b>3</b> | <b>-</b> | <b>-</b> | <b>-</b> |
|               |                              | <b>CO6</b>      | <b>-</b> | <b>-</b> | <b>-</b> | <b>-</b> | <b>-</b> | <b>3</b> | <b>3</b> | <b>3</b> | <b>-</b> | <b>-</b> | <b>-</b> |

# SEMESTER III

(Common Subjects for all Specializations)

|                          |  |
|--------------------------|--|
| <b>Course title/code</b> | <b>SYMMETRY &amp; GROUP THEORY (CHH 601B) [Common for all specialization]</b>                            |
| <b>Course Type</b>       | Core   |
| <b>Course Nature</b>     | Hard   |
| <b>L-T-P-O Structure</b> | 4-0-0-0  |
| <b>Objectives</b>        | To familiarize with Symmetry elements and symmetry operations<br>To impart knowledge on optical activity |
| <b>Outcome</b>           | Students will be able to understand group representation of various molecules.                           |
| <b>Prerequisites</b>     | Inorganic Chemistry-I & II   |

## SECTION A

**Molecular Symmetry:** Symmetry elements and symmetry operations, definition of group and its characteristics, subgroups, classes, similarity transformation. Products of symmetry operations,

equivalent atoms and equivalent symmetry elements, relations between symmetry elements and operations, classes of symmetry operations, point groups and classification. Symmetry: Optical activity and dipole moment

### SECTION B

**Representation of Groups:** Reducible and irreducible representations. The great Orthogonality theorem, character tables, position vector and base vector as basis for representation. Wavefunctions as bases for irreducible representations (p and d-orbitals). Direct product. Vanishing integral.

### SECTION C

**Coupling for Transition Metals:** Russell-Saunders coupling for  $d_n$  method of states. Splitting of one-electron levels in an octahedral environment. Correlation diagram. The method of descending symmetry, selection rules, Application of group theory to chemical bonding, hybridizations

### SECTION D

**Application of Group Theory:** Applications of group theory in Vibrational Spectroscopy: A brief idea about Infrared and Raman scattering spectroscopy. Vibrational modes as basis of group representations, Mutual exclusion principle, Classification of vibrational modes (i.e. stretching and angle deformation vibrations)

#### Books Recommended

1. F.A. Cotton; Chemical applications of Group Theory, 2<sup>nd</sup> ed. John Wiley & Sons, 1971
2. P. J. Durrant and B. Durrant, Introduction to Advanced Inorganic Chemistry, Longman, 1962
3. V. H. H. Jaffe and M. Orchin; Symmetry in Chemistry, John Wiley & Sons, New York, 1965

|                               |   |
|-------------------------------|---|
| <b>Course Title/<br/>Code</b> | <b>Scientific Research (RDO503) (COMMON FOR ALL SPECIALIZATIONS)</b>  |
| <b>Course Type</b>            | <b>Research &amp; Training</b>  |
| <b>Course Nature</b>          | Practical   |
| <b>L-T-P-O Structure</b>      | 0-0-8   |
| <b>Prerequisites</b>          | <b>Basic knowledge of Research</b>  |
| <b>Objectives</b>             | To acquaint the researcher with the tools of research by exposing them to the mechanics of writing a research report/ research paper/ thesis/ dissertation. |

|                          |   |
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| <b>Learning Outcomes</b> | <ol style="list-style-type: none"> <li>1. The student shall be able to describe research and its impact.</li> <li>2. The student shall be able to identify broad area of research, analyze, the processes and procedures to carryout research.</li> <li>3. The student shall be able to use different tools for literature survey</li> <li>4. The student is able choose specific area of research and supervisor/mentor is finalized</li> <li>5. To understand and adopt the ethical practice those are to be followed in the research activities</li> </ol> |
|--------------------------|---|

### **Unit 1: Importance of Research**

- 1.1 Capturing the current research trends
- 1.2 Insight about scientific research performed by renowned experts in the related field (case studies)
- 1.3 Do's and Don'ts pertaining to research
- 1.4 Identification of thrust area of research for deciding broad area
- 1.5 Framing the research questions and hypothesis
- 1.6 Identification of the research gap based on feasibility of problem
- 1.7 Exploration of in-house and commercially available facilities related to broad area

### **Unit 2: Literature Survey: Tools and Techniques**

- 2.1 Finding research papers related to a topic
- 2.2 Understanding the different aspects of Literature search
- 2.3 Usage of different sources like Google scholar, WoS, SCI/ SCIE, PubMed, Scopus, ABDC, EBSCO etc.
- 2.4 Search for online journals relevant to research area
- 2.5 Indexing of Journals
- 2.5 Usage of scholarly networking sites like Research Gate, Mendeley, and Academia.edu etc.
- 2.6 Demo sessions on the usage of above mentioned sources

### **Unit 3: Review of Literature and Identification of Gap**

- 3.1 Selection of relevant papers
- 3.2 Finding specific research problem from broad area of research
- 3.3 Literature survey and justification of specific research problem
- 3.4 Experimentation and data cleaning and verification
- 3.5 Understanding and selection of the research domain
- 3.6 Seeking information through published work w.r.t the problem
- 3.7 Reading & categorizing the downloaded/referred papers and structuring of the idea
- 3.8 Model design about framing the research questions

### **Unit 4: Report Writing and Presentation skill Development**

- 4.1 Report making on the surveyed literature to cater the basic idea of the research papers
- 4.2 Compiling and analyzing the published results to justify and understand the proposed ideas

- 4.3 Usage of MS-PowerPoint and other technical resources for the presentation
- 4.4 Development of presentation skills and group addressing
- 4.5 Scientific/technical writing and ethical practice, project report

**Evaluation Criteria for Scientific Research (Research Based)**

|              | <b>3rd Semester</b><br>Scientific Research RDO503   | <b>4th Semester</b>   |
|--------------|---|---|
| <b>Grade</b> | <b>Parameters of assessment for Research Publications</b>   | <b>Project</b>  |
| O /A+        | Depth of Research, Novelty of Topic<br>Relevance in Research, Proper Presentation & Literature Review Report (L.R.)                 | 1. Publication / Acceptance of paper in indexed journals<br>or<br>2. Conference papers in Scopus database etc. other than non-indexed proceedings |
| A / B+       | Average Presentation<br>Structured L.R. Depth of Research<br>Novelty of Topic<br>Relevance in Research<br>Proper Presentation & L.R | a) Published/ accepted in other referred list i.e UGC and other than databases like Scopus, WOS etc.  |
| B / C        | Average presentation<br>Moderate L. R.  | Published in non-referred journals  |
| C / P        | Faulty L.R. Poor presentation   | Ready to communicate/ paper presented in conference only  |
| F / Ab       | Unsatisfactory report / Absent  | Unsatisfactory report / absenteeism   |

**Note:-** In the above evaluation if the student adopts to join the industrial training in the final semester in Project work then the evaluation of the Scientific Research will be followed as mentioned above and the industrial training will be evaluated with the mid-term on spot /online/offline work presentation and final term training evaluation in the end of the training by a team of internal and external expert as mentioned in the regulation.

# SEMESTER III

(Physical Specialization)

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| <b>Course title/code</b> | <b>Physical Special I: Magneto-chemistry, Chemical Kinetics, Catalysis &amp; ion transport (CHH-602-B)</b>               |
| <b>Course Type</b>       | Domain Core  |
| <b>Course Nature</b>     | Hard   |
| <b>L-T-P-O Structure</b> | 4-0-0-0  |
| <b>Objectives</b>        | To impart knowledge of magnetochemistry<br>To impart advanced knowledge and application of kinetics and electrochemistry |
| <b>Outcome</b>           | Student will be able to  |



|                      |  |
|----------------------|--|
|                      | 1. understand the knowledge of magnetochemistry and its application<br>2. understand knowledge and applications of kinetics and electrochemistry |
| <b>Prerequisites</b> | Physical Chemistry-I & II  |

#### SECTION-A

**Magnetochemistry:** Magnetic susceptibility and its determination, susceptibility equivalents, Pascal's law and its applications, Diamagnetism of elements, Compounds and its ions, Langevin's theory of paramagnetism, Curie's law, Weiss molecular field theory of paramagnetism, Curie- Weiss law, Determination of Curie point.

#### SECTION-B

**Chemical Kinetics:** Kinetics of fast reactions: Techniques of study of fast reactions with reference to stop flow, T-Jump, Flash photolysis and relaxation phenomena. Kinetics of oscillating reactions with special reference to Belousov-Zhabotinskii mechanism (B-Z mechanism)

#### SECTION-C

**Catalysis & Kinetics:** a) Oxidation of sugars by  $K_3Fe(CN)_6$  and  $Cu^{+2}$  in alkaline medium, (b)Uncatalyzed and platinum group metals (Osmium, ruthenium, iridium, palladium, rhodium etc.) Catalyzed oxidation of organic and inorganic compounds by  $K_3Fe(CN)_6$  and Ce (IV) etc in acidic / alkaline medium.

#### SECTION-D

**Ion Transport in solutions:** Ionic movement under the influence of an electric field , mobility of ions, ionic drift velocity and its relation with current density, Einstein relation between the absolute mobility and diffusion coefficient, the Stokes- Einstein relation , the Nernst -Einstein equation, Waldens rule, the Rate- Process approach to ionic migration , the Rate process equation for equivalent conductivity, total driving force for ionic transport, Nernst - Planck Flux equation, ionic drift and diffusion potential , the Onsager phenomenological equations, The basic equation for the diffusion, Planck- Henderson equation for the diffusion potential

#### Reference Books

1. Peter Atkins & Julio De Paula, Physical Chemistry 10th Ed., Oxford University Press (2014).
2. G. W. Castellan, Physical Chemistry, 4th Ed., Narosa (2004).
3. G. A. McQuarrie, J. D. Simon, J. D., Molecular Thermodynamics, Viva Books Pvt. Ltd.: New Delhi (2004).
4. T. Engel, P. Reid, Physical Chemistry 3rd Ed., Prentice-Hall (2012).
5. M. J. Assael, A. R. H. Goodwin, M. Stamatoudis, W. A. Wakeham, S. Will, Commonly Asked Questions in Thermodynamics. CRC Press: NY (2011).
6. S. S. Zundhal, Chemistry concepts and applications Cengage India (2011).
7. D. W. Ball, Physical Chemistry Cengage India (2012).
8. R. G. Mortimer, Physical Chemistry 3rd Ed., Elsevier: NOIDA, UP (2009).
9. I. N. Levine, Physical Chemistry 6th Ed., Tata McGraw-Hill (2011).
10. C. R. Metz, Physical Chemistry 2nd Ed., Tata McGraw-Hill (2009).

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| <b>Course title/code</b> | <b>Physical Special II<br/>Irreversible thermodynamics, Transport Phenomenon, Photochemistry &amp; Fast Reaction (CHH 603B)</b> |
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| <b>Course Type</b>       | Domain Elective   |
| <b>Course Nature</b>     | Hard  |
| <b>L-T-P-O Structure</b> | 4-0-0-0   |
| <b>Objectives</b>        | To impart knowledge of Irreversible thermodynamics,<br>To impart advanced knowledge of transport phenomenon<br>To impart photochemistry & Fast reactions  |
| <b>Outcome</b>           | Student will be able to<br>1. understand the knowledge of Irreversible thermodynamics,<br>2. understand knowledge of transport phenomenon<br>3. understand knowledge of photochemistry & Fast reactions |
| <b>Prerequisites</b>     | Physical Chemistry-I & II   |

#### SECTION-A

**Irreversible thermodynamics** Meaning and scope of irreversible thermodynamics, Thermodynamic criteria for nonequilibrium states, Phenomenological laws- Linear laws, Gibbs equation, Onsager's reciprocal relations, Entropy production- specific examples of entropy production, Non-equilibrium stationary states, Prigogine's principle of maximum entropy production, Coupled phenomena. Some important applications of activation

#### SECTION-B

**Transport phenomena:** Diffusion coefficients, Fick's first and second laws, relation between flux and viscosity, relation between diffusion coefficient and mean free path, relation between thermal conductivity/viscosity and mean free path of a perfect gas, Einstein relation, Nernst-Einstein equation, Stokes-Einstein equation, Einstein-Smoluchowski equation.

#### SECTION-C

**Photochemistry:** Primary and secondary processes in photochemistry, Fate and properties of excited states, Photoluminescence and Photostationary state, Photosensitization, Rice – Herzfeld mechanisms. Photochemical chain reactions (hydrogen and chlorine, hydrogen and bromine) Non-chain photochemical reactions (formation of phosgene, decomposition of H<sub>2</sub>O<sub>2</sub> in presence of CO)

#### SECTION-D

**Fast reactions:** Luminescence and energy transfer processes, study of kinetics by stopped-flow technique, relaxation method, flash photolysis and magnetic resonance method, Kinetics of solid-state reactions size of a hole

#### Reference Books

1. Katchalsky, A. & Curren, P. F. *Non Equilibrium Thermodynamics in Biophysics* Harvard University Press: Cambridge (1965).
2. Kalidas, C. & Sangaranarayanan, M.V. *Non-Equilibrium Thermodynamics: Principles & Applications*, Macmillan India Ltd. (2002).
3. Laidler, K. J. *Chemical Kinetics* 3rd Ed., Benjamin Cummings (1997).
4. Thomas, J. M. & Thomas, M. J. *Principles and Practice of Heterogeneous Catalysis* John Wiley & Sons (1996).
5. Chorkendorff, Ib. & Niemantsverdriet, J. W. *Concepts of Modern Catalysis and Kinetics* Wiley-VCH (2003).
6. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).

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|--------------------------|---|
| <b>Course title/code</b> | <b>Physical Elective-I Advanced Spectroscopy (CHH 604 B)</b>  |
| <b>Course Type</b>       | Domain Elective   |
| <b>Course Nature</b>     | Hard  |
| <b>L-T-P-O Structure</b> | 4-0-0-0   |
| <b>Objectives</b>        | To impart knowledge of qualitative treatment of spectroscopic<br>To impart advanced knowledge and application of kinetics and electrochemistry                              |
| <b>Outcome</b>           | Student will be able to<br>1. understand the knowledge of magnetochemistry and its application<br>2. understand knowledge and applications of kinetics and electrochemistry |
| <b>Prerequisites</b>     | Physical Chemistry-I & II   |

#### SECTION-A

**Molecular Structure and Spectroscopy Spectroscopic methods:** Characterization of electromagnetic radiation, Born- Oppenheimer approximation, Heisenberg's Uncertainty Principle, Basic elements of spectroscopy, Time dependent perturbation, Einstein coefficients, Lambert-Beer's law, Integrated absorption coefficients, Transition dipole moments and general selection rules based on symmetry ideas

**Atomic spectra:** Characterization of atomic states, Microstate and spin factoring methods, Hund's rules, Derivation of spin and orbital selection rules (based on recursion relations of Legendre polynomials), Spectra of complex atoms, Zeeman and Stark effects, Atomic photoelectron spectroscopy,

#### SECTION-B

**Introduction to rotational spectroscopy:** Rotational spectroscopy of diatomic molecules based on rigid rotator approximation, Determination of bond lengths and/ or atomic masses from microwave data, Effect of isotopic substitution, Non-rigid rotator, Classification of polyatomic molecules, Energy levels and spectra of symmetric top molecules and asymmetric top molecules, First order Stark effect

**Vibrational spectroscopy:** Normal coordinate analysis of homonuclear and heteronuclear diatomic molecules, Extension to polyatomic linear molecules, Derivation of selection rules for diatomic molecules based on Harmonic oscillator approximation, Force constants and amplitudes. Anharmonic oscillator, Overtones and combination bands

#### SECTION-C

**Electronic spectroscopy:** Diatomic molecules, Selection rules, Breakdown of selection rules, Franck-Condon factors, Dissociation energies, Photoelectron spectroscopy of diatomic (N<sub>2</sub>) and simple polyatomic molecules (H<sub>2</sub>O, formaldehyde), Adiabatic and vertical ionization energies, Koopmans' theorem, Polyatomic molecules, Oscillator strengths, Use of Free Electron Model, HMO theory and Group theory for polyenes and carbonyl compounds (formaldehyde), Qualitative ideas of solvent effects- viscosity, polarity, hydrogen bonding

**Excited states:** Deactivation, Jablonskii diagram, Fluorescence and phosphorescence and factors affecting these calculations of excited state life-times from absorption data, Quenching of fluorescence, Stern-Volmer equation

#### SECTION-D

**NMR spectroscopy:** Larmor precession, Mechanisms of spin-spin and spin-lattice relaxations and quantitative treatment of relaxation, Quantum mechanical treatment of the AB system, Selection rules and relative intensities of lines

**Principles of Mossbauer spectroscopy:** Isomer shifts, Quadrupole and Nuclear Zeeman splittings, Applications in structure determination

#### Reference Books

1. Hollas. J. M. *Modern Spectroscopy* 4th Ed., John Wiley & Sons (2004).
2. Barrow, G. M. *Introduction to Molecular Spectroscopy* McGraw-Hill (1962).
3. Kakkar, R., *Atomic & Molecular Spectroscopy* Cambridge University Press (2015).
4. Brand, J. C. D. & Speakman, J. C. *Molecular Structure: The Physical Approach* 2nd Ed., Edward Arnold: London (1975).
5. Chang, R. *Basic Principles of Spectroscopy* McGraw-Hill, New York, N.Y. (1970).
6. Moore, W. J. *Physical Chemistry* 4th Ed. Prentice-Hall (1972).
7. Warren, B. E. *X-Ray Diffraction* Dover Publications (1990).
8. Bacon, G. E. *Fifty Years of Neutron Diffraction* Hilger (1987).

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|--------------------------|--|
| <b>Course title/code</b> | <b>Physical Elective-II<br/>Advanced Chemical Kinetics (CHH 605 B)</b>         |
| <b>Course Type</b>       | Domain Elective  |
| <b>Course Nature</b>     | Hard   |
| <b>L-T-P-O Structure</b> | 4-0-0-0  |
| <b>Objectives</b>        | To impart knowledge advanced chemical kinetics                                 |
| <b>Outcome</b>           | Student will be able to understand the knowledge of advanced chemical kinetics |
| <b>Prerequisites</b>     | Physical Chemistry-I & II  |

#### SECTION-A

**Statistical theories of kinetics:** Collision theory, Activated Complex theory, Potential energy surfaces- attractive and repulsive forces, Lindemann's theory of unimolecular reactions energy transfer, fall-off region and its limitations, Rice-Ramsperger and Kassel (RRK) model, and Marcus refinement of RRK model (RRKM) for the calculation of rate constants of simple unimolecular (isomerization) reactions.

#### SECTION-B

**Enzyme kinetics:** Michaelis-Menten mechanism - single and double intermediates, King- Altman method for working out the kinetics of complex enzyme reactions

**Enzyme inhibition-** reversibility and products inhibition, Computer simulation in chemical kinetics

#### SECTION-C

**Reaction Dynamics I:** Molecular beams, principle of crossed-molecular beams, Molecular encounters and principal parameters, e.g. Impact parameter, Collision cross-section, Reaction cross-section and relation between reaction cross-section and reaction rate (single velocity), Dependence of collisional cross-section on translational energy

#### SECTION-D

**Reaction Dynamics II:** Probing the transition state, Dynamics of barrier less chemical kinetics in solution, dynamics of unimolecular reactions and bimolecular reactions

#### Reference Books

1. Pilling, M. J. & Seakins, P. W. *Reaction Kinetics* Oxford Press (1997).
2. Laidler, K. J. *Chemical Kinetics* 3rd Ed., Benjamin Cummings (1997).

|                          |   |
|--------------------------|---|
| <b>Course title/code</b> | <b>Physical Laboratory (CHH 606B)</b>   |
| <b>Course Type</b>       | Core  |
| <b>Course Nature</b>     | Hard  |
| <b>L-T-P-O Structure</b> | 0-0-8-0   |
| <b>Objectives</b>        | To make student able to understand the practical aspects of kinetics of the reactions & different potentiometric titrations   |
| <b>Outcome</b>           | Student will be able to the exposure of practical aspects of kinetics of the reactions & different potentiometric titrations.<br>Student will be able to understand the research and experimental outcome analysis. |
| <b>Prerequisites</b>     | Laboratory work-II  |

### List of Experiments

1. Determine the concentration or percentage of one or two optically active substances in the given solution polarimetrically.
2. Kinetics of oxidation of reducing sugars by potassium ferricyanide/ copper(II) in presence of ammonium hydroxide or sodium hydroxide.
3. Kinetics of oxidation of alcohols/diols by aqueous alkaline hexacyanoferrate (III) ions.
4. Potentiometric titration of weak/strong acid and strong /weak base.
5. Study of the oxidation of cyclic alcohols by cerium(IV) sulphate in acidic medium in presence of Iridium(III) chloride.
6. Kinetics of iridium (III) catalyzed oxidation of aromatic aldehydes/aromatic alcohols/hydrocarbons by cerium (IV) in aqueous acidic medium.
7. Kinetics of Ru(III) catalysed oxidation of alcohols/diols by Ce(IV) sulphate in acidic medium .
8. Kinetics of oxidation of aliphatic/cyclic alcohols/glycols by alkaline hexacyanoferrate(III) catalyzed by ruthenium (III) chloride

# SEMESTER III

## (Inorganic Chemistry Specialization)

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| <b>Course title/code</b> | <b>Inorganic Special-I<br/>Organometallic Chemistry of Transition Metals &amp; Bio Inorganic Chemistry (CHH 608B)</b>   |
| <b>Course Type</b>       | Domain Core   |
| <b>Course Nature</b>     | Hard  |
| <b>L-T-P-O Structure</b> | 4-0-0-0   |
| <b>Objectives</b>        | To conceptualize the concept of bonding between organic ligands and transition metals.<br>To Understand physical and chemical properties of various classes of organometallic compounds.<br>To understand role of metal ions on biological system.<br>To apply the knowledge of metal toxicity in development of chelating agents for metal detoxification. |

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| <b>Outcome</b>       | The student will be able to extent applications of organometallic compounds in catalysis, and other industrial processes.<br>The student will be able to understand the use of Transition Metal Compounds in biological system. |
| <b>Prerequisites</b> | Inorganic Chemistry-I & II  |

### SECTION A

**Organometallic compounds-I:** Introduction, Stable electron configurations, Electron count preference, Electron counting and oxidation states, Nomenclature.

Ligands: Carbon monoxide, Phosphines, Hydrides and dihydrogen complexes, Alkyl, alkenyl, alkynyl, and -aryl ligands, Alkene and alkyne ligands, Nonconjugated diene and polyene ligands. Butadiene, cyclobutadiene and cyclooctatetraene, Benzene and other arenes, The allyl ligand, Cyclopentadiene and cycloheptatriene, Carbenes, Alkanes, agostichydrogens, and noble gases, Dinitrogen and nitrogen monoxide

### SECTION B

**Organometallic compounds-II:** d-Block carbonyls (Preparation, Properties), Metallocenes, Metal - Metal bonding and metal clusters. Reactions: Ligand substitution, Oxidative addition and reductive elimination,  $\sigma$  -Bond metathesis, 1,1-Migratory insertion reactions, 1,2-Insertions and  $\beta$  -hydride Elimination, Nucleophilic and Electrophilic attack, Hydride eliminations and cyclometallations

### SECTION C

**Bio-Inorganic Chemistry-I:** Fundamentals of inorganic biochemistry, geo-chemical effects on life systems, essential and non-essential elements in bio-systems. Role of alkali/alkaline earth metals in bio-systems, Role of 3d block elements and nonmetals in bio-systems, Role of metal ions in oxygen carriers and synthetic oxygen carriers. Designing of chelating agents and metal chelates as medicines, Fixation of dinitrogen biologically and abiotically, biotransformation of nonmetallic inorganic compounds, Environmental bioinorganic chemistry, Metal ions as probes for locating active sites, Biocatalysts

### SECTION D

**Bio-Inorganic Chemistry-II:** Inhibitions as competitive and non-competitive, metals and metalloproteins, Metal complexes of polynucleotides, nucleosides and nucleic acids (DNA & RNA), Templatetemperature, stability of DNA, Role of metal ions in replication and transcription process of nucleic acids, Biochemistry of di oxygen, bioinorganic chips and biosensors, Biochemistry of calcium as hormonal messenger, muscle contraction blood clotting, neurotransmitter, calcification reclaiming of barren land. Cytochromes, ferredoxins and ironsulphur proteins, ion transport across membranes, Biological nitrogen fixation, PSI, PS – II, Oxygen uptake proteins

### Reference Books

1. Bioinorganic Chemistry Williams, An Introduction to Bioinorganic Chemistry
2. M. N. Hughes, Inorganic Chemistry of Biological Processes
3. Ochiai: Bioinorganic Chemistry: Allyn & Bacon Burton
4. P. L. Pauson, Organometallic Chemistry
5. T. S. Swain and D. S. T. Black, organometallic Chemistry
6. Eichhorn: Inorganic Biochemistry : Vol I , 2 Elsevier

7. Williams: an Introduction to Bioinorganic Chemistry, C.C. Thomos Spring III
8. Wallace: Decade on synthetic chelating agent in Inorganic plant nutrition, Wallace

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|--------------------------|---|
| <b>Course title/code</b> | <b>Inorganic Special-II: Supramolecular Chemistry &amp; Metal Clusters (CHH 609B)</b>   |
| <b>Course Type</b>       | Domain Core   |
| <b>Course Nature</b>     | Hard  |
| <b>L-T-P-O Structure</b> | 4-0-0-0   |
| <b>Objectives</b>        | To conceptualize the concept of supramolecular interactions, macrocyclic compounds and template synthesis<br>To Understand chemical properties of cages, metal clusters, carboranes, phosphazies.<br>To understand role of silicates and aluminosilicates<br>To conceptualize the concept of clays, zeolites and its applications |
| <b>Outcome</b>           | The student will be able to extent applications of supramolecular molecules and other industrial process<br>The student will be able the understand the use of zeolites, clays, silicates, aluminosilicates in industrial appliatications.  |
| <b>Prerequisites</b>     | Inorganic Chemistry-I & II  |

#### SECTION A

**Supramolecular Chemistry-I:** Molecules and Supramolecules, Supermolecules, Large Molecules Classification, Nomenclature, Thermodynamic and Kinetic selectivity, Supramolecular interactions, Supramolecular host design, Macrocyclic versus acyclic hosts, Chelate Macrocyclic and macrobicyclic hosts, High dilution synthesis, Template synthesis

#### SECTION-B

**Supramolecular Chemistry-II:** Molecular recognition: Receptors, design and synthesis of co-receptors and multiple recognition, Hydrogen bonds, strong, weak and very weak H-bonds, Utilisation of H-bonds to create supramolecular structures, Use of H-bonds in crystal engineering and molecular recognition, Chelate and macrocyclic effects.

#### SECTION C

**Chemistry of Inorganic Rings, Cages and Metal Cluster Compounds-I:** Chemistry of inorganic rings, cages and metal cluster compounds, borazines, phosphazenes, polyhedral boranes, carboranes, metalloboranes and metallocarboranes  
Silicates and aluminosilicates: Classifications, structure, properties and applications of naturally occurring silicates and aluminosilicates.

#### SECTION D

**Chemistry of Inorganic Rings, Cages and Metal Cluster Compounds-II:** Syntheses of pillared clays and zeolites, Characterization of clays, pillared clays and zeolites from measurement of surface area, surface activity pore size, distribution and interlayer spacing, Application of clays, pillared clays and zeolites with emphasis of catalyses

#### Reference Books

1. Ballhausen C. J. *Introduction to Ligand Field Theory* McGraw Hill Book Co.: N.Y (1962).



2. Marshal, C. E. *The Physical Chemistry and Mineralogy of Soil Vol. I Soil Materials* John Wiley & Sons.
3. Wells, A. F. *Structural Inorganic Chemistry* Oxford University Press.
4. Adams, D. M. *Inorganic Solids. An Introduction to Concepts in Solid-State Structural Chemistry* John Wiley & Sons
5. Azaroff, L. V. *Introduction to Solids* Tata McGraw Hill Publishing Co. Ltd.
6. Breck, D. W. *Zeolites Molecular Sieves- Structure, Chemistry and Use.* John Wiley & Sons.

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|--------------------------|---|
| <b>Course title/code</b> | <b>Inorganic Special-Elective: Solid state Materials (CHH 610B)</b>   |
| <b>Course Type</b>       | Domain Elective   |
| <b>Course Nature</b>     | Hard  |
| <b>L-T-P-O Structure</b> | 4-0-0-0   |
| <b>Objectives</b>        | To familiarize students with the concept of solids, their properties, preparation methods, etc. To gain the knowledge of the chemistry between layered structures of solids |
| <b>Outcome</b>           | Students will be able to understand the structural aspects of inorganic solid substance and properties associated with different solid structures.                          |
| <b>Prerequisites</b>     | Inorganic Chemistry I and II  |

#### Section A

**Electronic, Electric and Optical behaviour of Inorganic materials:** Electronic structure of solids, band theory, band structure of metals, insulators and semiconductors, the band gap, Intrinsic and extrinsic semiconductors, doping of semiconductors and conduction mechanism, temperature dependence of conductivity, carrier density and carrier mobility in semiconductors, synthesis and purification of semiconducting materials, single crystal growth, rectifier transistors, optical devices

#### Section B

**Methods to synthesize solid-state materials:** Ceramic method, solid-state reaction and its kinetics, hydrothermal, sol-gel, co-precipitation (precursor), vapor phase transport methods.

**Amorphous inorganic materials:** Glasses, refractories, materials obtained from organometallic chemical vapor deposition (MOCVD)

#### Section C

**Inorganic Polymers:** Classification, types of Inorganic polymers, Chemistry of following polymers a) Silicones b) phosphonitric halides c) condensed phosphates d) coordinated polymers e) Silicates f) Isopoly & heteropoly acids

**Solid State lasers (Ruby, YAG and tunable lasers):** Inorganic Phosphor materials, synthesis and advantages of optical fibers, over conducting fibers

#### Section D

**Mesoporous materials and their catalytic applications:** Various types of mesoporous materials (oxides, sulphides), tailoring of pore size, applications of mesoporous materials in heterogeneous catalysis

**Intercalation chemistry:** Introduction, intercalation reactions in graphite, layered double hydroxides, layered sulfides, applications of intercalation chemistry

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| <b>Course title/code</b> | <b>Inorganic Elective: Inorganic and Biological Catalysis (CHH 611B)</b> |
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| <b>Course Type</b>       | Domain Elective  |
| <b>Course Nature</b>     | Hard   |
| <b>L-T-P-O Structure</b> | 4-0-0-0  |
| <b>Objectives</b>        | To conceptualize the concept of catalyst and their importance in industrial applications<br>To understand the concept of toxicology and detoxification in biological systems.  |
| <b>Outcome</b>           | The student will be able to extend applications of inorganic catalyst in various industries<br>The student will be able to understand the use of inorganic and biological catalyst in various biochemical reactions. |
| <b>Prerequisites</b>     | Inorganic I & II   |

### SECTION A

**Catalysis I:** ligands in homogeneous catalysis such as CO, amines, phosphines, NHC's, alkenes, alkynes, carbenes, carbynes, etc. General principles, Homogeneous Catalysis (alkene metathesis, Types of metathesis such as RCM, ROM, ROMP, ADMET and EM hydrogenation of alkenes, hydroformylation, Wacker oxidation on alkenes, asymmetric oxidation, methanol carbonylation.

### SECTION B

**Catalysis II:** Heterogeneous catalysis (nature of heterogeneous catalysts, hydrogenation catalysts, catalytic cracking), electrocatalysis, Hybrid Catalysis. Grubbs I, II and III, Schrock and Schrock-Hoveyda catalysts, Fischer-Tropsch process, C-H activation of alkyls and aryls using transition metal complexes.

### SECTION C

**Catalysis III:** Applications in Industry: Palladium and Nickel catalyzed cross-coupling reactions such as Suzuki, Heck, Sonogashira, Stille Coupling, Negishi, Hiyama coupling, Buchwald-Hartwig, decarboxylative cross-coupling and alpha arylation of carbonyls.

### SECTION-D

**Toxicology:** Metal poisoning and treatment by using chelating agent, mercury, lead & cadmium poisoning & treatment. Metals in the regulation of biochemical events, Transport and storage of metal ions in vivo. Biochemistry of calcium as hormonal messenger, and neurotransmitter. Fundamentals of toxicity and detoxification.

### Reference Books

1. Principles of Bioinorganic chemistry, S. J. Lippard and J. M. Berg
2. Bioinorganic chemistry, I. Bertini, H. B. Gray, S. J. Lippard, and J. S. Valentine
3. Progress in inorganic chemistry Vol. I and Vol. II .ed. G. L. Eichorn, Elsevier
4. Progress in inorganic chemistry Vols 18 and 38 ed. J. J. Lippard, Wiley.

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|--------------------------|--|
| <b>Course title/code</b> | <b>Inorganic Laboratory (CHH 612B)</b>   |
| <b>Course Type</b>       | Core   |
| <b>Course Nature</b>     | Hard   |
| <b>L-T-P-O Structure</b> | 0-0-8-0  |
| <b>Objectives</b>        | To impart the laboratory exposure to the synthesis of coordination complexes and quantitative analysis of the inorganic mixtures |
| <b>Outcome</b>           | Students will be able to hands on laboratory exposure to the synthesis of coordination complexes                                 |

|                      |   |
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|                      | and quantitative analysis of the inorganic mixtures |
| <b>Prerequisites</b> | Physical Chemistry-I & II                           |

### List of Experiments

- Quantitative separations and determinations of following pairs of metal ions using gravimetric and volumetric methods
 

|                                     |                                     |                                     |                                     |
|-------------------------------------|-------------------------------------|-------------------------------------|-------------------------------------|
| (a) $\text{Ag}^+/\text{Cu}^{2+}$    | (b) $\text{Cu}^{2+}/\text{Zn}^{2+}$ | (c) $\text{Fe}^{3+}/\text{Ca}^{2+}$ | (d) $\text{Ba}^{2+}/\text{Cu}^{2+}$ |
| (e) $\text{Ni}^{2+}/\text{Zn}^{2+}$ | (f) $\text{Ag}^+/\text{Ni}^{2+}$    | (g) $\text{Fe}^{3+}/\text{Ni}^{2+}$ |                                     |
- Inorganic Preparations of the following compounds
  - Prussian Blue
  - Trisacetylacetonato Iron (III)
  - Tetraammine copper (II) sulphate monohydrate
  - Hexamine cobalt (III) hexanitritocobaltate (III)
  - Sodium hexanitritocobaltate (III)

### Reference Books

- J. Singh, R. K. P. Singh, J. Singh, L. D. S. Yadav, I. R. Siddiqui and J. Srivastava; Advanced Practical Chemistry, 2<sup>nd</sup> ed. PragatiPrakashan, 2010
- A. I. Vogel; Vogel's textbook of Practical Inorganic Analysis, 5<sup>th</sup> ed. Longman Scientific and technical Publisher, UK, 1989

# SEMESTER III

## (Organic Specialization)

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|--------------------------|---|
| <b>Course title/code</b> | <b>Organic Special-I: Statistical Stereochemistry &amp; Asymmetric Synthesis (CHH 613B)</b>   |
| <b>Course Type</b>       | Core  |
| <b>Course Nature</b>     | Hard  |
| <b>L-T-P-O Structure</b> | 4-0-0-0   |
| <b>Objectives</b>        | To impart the knowledge of stereochemistry of the organic molecules.<br>To impart the knowledge of various methods of asymmetric synthesis  |
| <b>Outcome</b>           | Student will be able to<br>1. Understand the nomenclature, configuration and stereochemistry of cyclic and acyclic molecules.<br>2. Understand the various methods of to induce asymmetry in the molecules. |
| <b>Prerequisites</b>     | Organic Chemistry-I & II  |

### SECTION A

**Stereochemistry-I:** Configurational Isomerism (optical and geometrical), Resolvable and non-resolvable compounds, Geometrical isomerism (single bond, multiple bond and monocyclic, bicyclic, bridging and polycyclic structure), and threo-erythro nomenclature, representation and interconversion of Fischer, Newman, Sawhorse and flying wedge formulae, Relative and absolute configuration, Epimers and anomers

#### SECTION B

**Stereochemistry-II:** Relationship between the molecules: homologues, conformational, configurational, epimers, anomers, geometrical, optical, enantiomers, identical, diastereomers etc. Axis of chirality and plane of chirality (ANSA compounds, p-cyclophanes, transcyclooctene), optical isomerism in allenes, biphenyls (atropoisomerism), bipyrrolles, binaphthols, spiranes, hemispiranes. elementary ideas about stereochemistry of tertiary amines, quaternary salts, sulphur and phosphorous compounds.

#### SECTION C

**Stereochemistry-III:** Topicity of ligands, lone pairs and faces, their nomenclature and prochiralcentre. Stereospecific and stereoselective reaction. Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry, substitution and addition criteria. . Prochirality nomenclature: Pro-R, Pro-S, Re and Si. Stereoselective reactions: Substrate stereoselectivity, product stereoselectivity, enantioselectivity and diastereoselectivity. Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Analytical methods: % Enantiomeric excess, enantiomeric ratio, optical purity, % diastereomeric excess and diastereomeric ratio.

#### SECTION D

**Methodologies in Asymmetric Synthesis:** Strategies in Asymmetric Synthesis:

**1.Chiral substrate controlled:** Nucleophilic additions to chiral carbonyl compounds (Cram's rule),  $\alpha$ -alkylation through oxazolines and azaenolates,  $\alpha$ -alkylation using imines, Ender's asymmetric  $\alpha$ -alkylation of hydrazones of aldehydes and ketones,

**2.Chiral auxiliary controlled:** 1, 4 Asymmetric induction (Prelog's rule),  $\alpha$ -alkylation of amino acids via imidazolidinones,  $\alpha$ -alkylation of  $\alpha$ -hydroxyl acids via lactones, asymmetric  $\alpha$ -alkylation of glycine, Evans alkylation of S-prolinol

**3.Chiral reagent controlled:** enantioselective hydroboration i.e. use of chiral boronhydrides (hydroborations with diisopinocampheylborane and hydroborations with monoisopinocampheylborane) and Chiral trialkylboranes (Midland's reagent)

**4.Chiral catalyst controlled:** Jacobsen epoxidation, homogenous hydrogenation, Chiral Ru and Rh catalysts for homogenous asymmetric hydrogenation.

#### Reference Books

1. Jonathan Clayden, Nick Greeves, Stuart Warren, Organic Chemistry, Oxford University Press, second edition
2. D. Nasipuri, Stereochemistry of Organic Compounds-Principles & Applications, New Age International.
3. P.S. Kalsi, Stereochemistry of Organic Compounds- Conformation and Mechanism: New Age International.
4. Ernest L Eliel & Samuel H. Wilen, Stereochemistry of Carbon compounds.
5. R S Ward, Stereo selectivity in organic synthesis
6. Howard, S. I.; Morrison, J. D. Asymmetric Synthesis; Academic: New York. 1983; Vol. 2.

7. Nogradi. M. Stereoselective Synthesis.

|                          |   |
|--------------------------|---|
| <b>Course title/code</b> | <b>Organic Special-II: Photochemistry And Pericyclic Reaction (CHH 614B)</b>  |
| <b>Course Type</b>       | Core  |
| <b>Course Nature</b>     | Domain  |
| <b>L-T-P Structure</b>   | 4-0-0-0   |
| <b>Objectives</b>        | The student will be exposed to photochemistry of various electronic transitions<br>The student will be introduced to various pericyclic reactions and their mechanisms                              |
| <b>Outcome</b>           | The student will be able to write mechanism of various pericyclic reactions.<br>Student will understand photochemistry of various electronic transition ( $\pi\text{-}\pi^*$ and $n\text{-}\pi^*$ ) |
| <b>Prerequisites</b>     | Organic Chemistry-I & II  |

### Section-A

**Photochemistry Of ( $\pi\text{-}\pi^*$ ) Transitions:** Excited states of alkenes, cis-trans isomerisation, photostationary state, electrocycloisatation and sigmatropic rearrangements, di- $\pi$  methane rearrangement. Intermolecular reactions, photocycloadditions, photodimerisation of simple and conjugated olefins, addition of olefins to  $\alpha$ ,  $\beta$ -unsaturated carbonyl compounds, excited states of aromatic compounds, Photoisomerisation of benzene

### SECTION-B

**Photochemistry of ( $N\text{-}\pi^*$ ) Transitions:** Excited states of carbonyl compounds, homolytic cleavage of  $\alpha$ - bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkanediones, Intermolecular abstraction of hydrogen: photoreduction - influence of temperature, solvent, nature of hydrogen donor and structure of the substrate Intramolecular abstraction of hydrogen: Norrish type II reactions in ketones, Esters and 1, 2- diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction, Photochemistry of nitrites-Barton reaction.

### SECTION-C

**Pericyclic Reactions I Introduction** - Characteristics and classification of pericyclic reactions— Electrocyclic, cycloaddition & cycloreversions and sigmatropic reactions— $4n$ e and  $4n+2$ e type examples, Approaches for the interpretation of mechanism of pericyclic reactions—Aromatic Transition States (ATS)/Perturbation, Molecular Orbitals (PMO) approach—Concept of Huckel – Mobius aromatic and antiaromatic transition states, Framing Woodward-Hofmann selection rules for all the pericyclic reactions by ATS approach, Solving problems based on ATS approach.

### SECTION-D

**Pericyclic Reactions II:** Molecular orbitals—definition and their origin—Non-mathematical writing up of molecular orbitals and their symmetry properties for acyclic conjugated systems, Frontier Molecular Orbital (HOMO LUMO) approach—concept—Framing Woodward-Hofmann selection rules for all the pericyclic reactions by Frontier Molecular Orbital (FMO) approach, Solving problems based on FMO approach, Conservation of orbital symmetry (Correlation Diagrams) approach—concept— Framing Woodward-Hofmann selection rules for electrocyclic and cycloadditions & cycloreversions by Conservation of orbital symmetry approach.

### Reference Books

1. J. Singh and J. Singh; Photochemistry and Pericyclic reactions, 3<sup>rd</sup>ed. New Age International Pvt Ltd, 2005
2. S. Sankararaman; Pericyclic Reactions- A text Book, 1<sup>ST</sup> ed. Wiley VCH, 2005

3. W. Horsepool; Handbook of Organic Photochemistry and Photobiology, 1<sup>st</sup> ed. CRC Press, 1984

|                          |  |
|--------------------------|--|
| <b>Course title/code</b> | <b>Organic Special-Elective: Modern Organic Synthetic Technique (CHH 615B)</b>   |
| <b>Course Type</b>       | Core   |
| <b>Course Nature</b>     | Elective   |
| <b>L-T-P-O Structure</b> | 4-0-0-0  |
| <b>Objectives</b>        | To familiarize the student with the various synthetic reagents for using group protection and oxidation reactions. To make the student understand the mechanism of various synthetic routes.<br>To make the student understand the new techniques and concepts in organic synthesis<br>Student will be familiarized with stereochemistry principles. |
| <b>Outcome</b>           | The student will be able to write the mechanism of organic reactions. The student will be able to predict the structure of organic compounds by stereochemistry.   |
| <b>Prerequisites</b>     | Organic Chemistry-I & II   |

#### SECTION A

**Hybrid Transfer Reagents:** Sodium borohydride, lithium aluminum hydride and alkoxy substituted LAH reducing agents, DIBAL,

**Common Named Reactions And Rearrangements** – applications in organic synthesis

**Name Reaction:** Appel, Birch, Cannizzaro, Claisen, Clemmensen, Curtius, Dakin-West, Eschweiler-Clarke, Finkelstein, Gabriel, Heck, Mannich, Negishi cross-coupling, Prins, Ritter, Stille, Suzuki, Sonogashira coupling, Swern, Ullman, Wittig Reactions

**Rearrangement:** Beckmann, Curtius, The Lossen, Baeyer-Villiger, Favorskii, Fries, Claisen, Benzilic acid, Wagner Meerwein rearrangement, Pinacol-pinacolone rearrangements and Wolf Rearrangement

#### SECTION B

**Redox Reactions: Oxidation** - Introduction, Different oxidative processes for the followings: Hydrocarbons- alkenes, aromatic rings, saturated C-H groups (activated and unactivated). Alcohols, diols, aldehydes, ketones, and carboxylic acids

**Reduction** – Introduction, Different reductive processes for followings: Hydrocarbons – alkanes, alkenes, alkynes and aromatic rings. Carbonyl compounds – aldehydes, ketones, acids and their derivatives. Nitro compounds.

#### SECTION C

**Newer Synthetic Reactions and Reagents:** Enolates, enolate equivalents and enamines: Applications in carbon-carbon bond formation and related reactions.

**Phosphorus, Sulphur and nitrogen ylides:** Preparation, applications in organic synthesis and mechanism.

**Principles and applications** of phase transfer catalysis, crown ethers and polymer-supported reagents in organic synthesis.

#### SECTION D

**Philosophy of organic synthesis:** Disconnection approach, one group and two group disconnections, reversal of polarity, chemoselectivity, one group C-C disconnection, two group C-C disconnections, 1,3-difunctional and 1,5-difunctional compounds. **Umpolung reactions** (sulphur compounds, nitro compounds, lithiated ethers and related compounds).

### Reference Books

1. I.M. B. Smith and Jerry March; March's Advanced Organic Chemistry, 5<sup>th</sup> ed. John Wiley & Sons, New York, 2001
2. F. A. Carey and R. J. Sundberg; Advanced Organic Chemistry, 5<sup>th</sup> ed. Springer Publishers, 2008
3. R.T. Morrison and R.N. Boyd; Organic Chemistry, 6<sup>th</sup> ed. Prentice Publishing, 1992
4. H. O. House, W. A. Benjamin; Modern Organic Reactions, 2<sup>nd</sup> ed. VCH Publishers, USA, 1972
5. R. O. C. Norman and J. M. Coxon; Principles of Organic Synthesis, 3<sup>rd</sup> ed. Blackie Academic & Pro, 1993
6. S. M. Mukherji and S. P. Singh; Reaction Mechanism in Organic Chemistry, 3<sup>rd</sup> ed. Macmillan, 1984

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|--------------------------|--|
| <b>Course title/code</b> | <b>Organic Special-Elective: Bioorganic Chemistry (CHH 616B)</b>   |
| <b>Course Type</b>       | Core   |
| <b>Course Nature</b>     | Elective   |
| <b>L-T-P-O Structure</b> | 4-0-0-0  |
| <b>Objectives</b>        | To impart the knowledge of the activity of the organic biomolecules and its applications in biological systems         |
| <b>Outcome</b>           | Student will be able to understand the activity of the organic biomolecules and its applications in biological systems |
| <b>Prerequisites</b>     | <b>Organic Chemistry-I &amp; II</b>  |

### SECTION-A

**Enzymes and Their Action:** Introduction to enzymes. Transition state theory, Acid-Base catalysis, Covalent catalysis— Binding modes of catalysis (i) Proximity effect (ii) Transition state stabilization (iii) Strain and Distortion. Examples of some typical enzyme mechanisms for (1) Triose phosphate isomerase, (ii)  $\alpha$ -chymotrypsin and serine protease (iii) Lysozyme (iv) Carboxy peptidase-A (v) Ribonuclease.

### SECTION-B

**Enzyme Models & Enzymatic Transformations:** Introduction — Biomimetic chemical approach to biological systems—Enzyme models Advantage of enzyme models, Requirements necessary for the design of enzyme models, Host-Guest complexation chemistry, Examples of some host molecules—Crown ether cryptanes, cyclodextrins, Cyclodextrin based enzyme models—Valixarenes, ionophores, micelles and synzymes (synthetic enzymes) — chiral recognition and catalysis. Introduction to industrial enzymes, Enzymatic synthesis of  $\alpha$ -amino acids and peptides, Transformations of lipases and esterases, Kinetic resolutions of carboxylic acids, esters and alcohols – Transesterification, Amine resolution—use of oxido-reductase, C-C bond formation using enzymes—asymmetric cyanohydrin formation and asymmetric aldol condensations

### SECTION-C

**Recombinant DNA and Fermentation Technology:** Introduction to genetic engineering. Recombinant DNA technology—restriction endonuclease, cloning, linkers, adaptors, Application of recombinant DNA technology in production of pharmaceuticals, diagnosis of diseases, insect control, improved biological detergents, gene therapy—examples, Principles of finger printing technology—Site directed mutagenesis.



**FERMENTATION TECHNOLOGY:** Introduction to fermentation. Industrial fermentation, Advantages and limitations of fermentation, Production of drugs and drug intermediates from fermentation examples, Chiral hydroxy acids, vitamins, amino acids,  $\beta$ -lactam antibiotics, Precursor fermentation and microbial oxidation and reductions.

#### SECTION-D

**COENZYMES:** Introduction, Co factors — cosubstrates — prosthetic groups. Classification — Vitamin derived coenzymes and metabolite coenzymes. Structure and biological functions of coenzyme, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of i) nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, NADP<sup>+</sup> NADPH ii) Flavin adenine nucleotide FAD, FADH<sub>2</sub> and iii) Flavin mononucleotide (FMN, FMNH<sub>2</sub>) lipoic acid, biotin, tetrahydrofolate and ubiquinone, Adenosine triphosphate (ATP) and adenosine diphosphate (ADP), S-adenosyl methionine (SAM) and uridine diphosphate sugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes.

#### Reference Books:

I. L. Finar; Organic Chemistry, Vol. II, 5<sup>th</sup> ed. Pearson Education, 1956

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|--------------------------|--|
| <b>Course title/code</b> | <b>Organic Special-Elective: Chemistry of Natural Products (CHH 617B)</b>  |
| <b>Course Type</b>       | Core   |
| <b>Course Nature</b>     | Elective   |
| <b>L-T-P-O Structure</b> | 4-0-0-0  |
| <b>Objectives</b>        | To impart knowledge on Biosynthesis of natural products. To familiarize with Structure determination and stereochemistry of natural products by chemical methods and spectroscopic methods |
| <b>Outcome</b>           | Students will be able to write Biosynthesis of natural products. Students will be able to elucidate the structure of natural products by various spectroscopic techniques                  |
| <b>Prerequisites</b>     | <b>Organic I &amp; II</b>  |

#### SECTION-A

**Biosynthesis of secondary metabolites:** Introduction to natural products, Synthesis and Biosynthesis (similarities & differences), Biogenesis, Primary and secondary metabolites, Why plants produce secondary metabolites, Characteristics of secondary metabolites, Biosynthesis of natural products (schematic representation), methods of investigation of biosynthesis of secondary metabolites, Reactions involved in biosynthesis (primary and secondary biosynthesis);

Biosynthesis of Acetyl CoA: biosynthesis by oxidative decarboxylation, Activation of acetic acid, properties (formation of malonyl CoA); Origin of aromatic ring in secondary metabolites (Shikimic acid pathway); Biosynthesis of terpenes (NPP, GPP, citral,  $\alpha$ -pinene,  $\alpha$ -terpineol, borneol); Biosynthesis of steroids (cholesterol), Biosynthesis of alkaloids: formation of alkaloid derived from phenylalanine-ephedrine, Biosynthesis of piperidine alkaloid-coniine, biosynthesis of pyrrolidine-pyridine alkaloid-nicotine, biosynthesis of tropane alkaloid-atropine, biosynthesis of cinchona alkaloid-quinine. Biosynthesis of fatty acids

#### SECTION-B

**Terpenoids & Carotenoids: Terpenoids:** Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Isolation of terpenes, Structure determination,

Monoterpenoids: Citral, geraniol (acyclic),  $\alpha$ -terpeneol, menthol (monocyclic), Sesquiterpenoids: Farnesol (acyclic), zingiberene (monocyclic), santonin (bicyclic), Diterpenoids: Phytol and abietic acid.

**Carotenoids:** General methods of structure determination of Carotenes:  $\beta$ - carotene, lycopene

### SECTION-C

**Alkaloids:** Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure and synthesis of the following: Ephedrine, Coniine, Nicotine, Atropine, Quinine and Morphine

### SECTION-D

**Steroids:** Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Androsterone, Testosterone, Progesterone

**Plant Pigments:** Occurrence, nomenclature and general methods of structure determination, Isolation and synthesis of Anthocyanins (Cyanin and pelargonidin), polyphenols: Flavones (chrysin), Flavonols (quercetin) and isoflavones (daidzein) coumarin, Quinones (lapachol), Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway

#### Books Recommended:

1. J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthrope and J. B. Harborne; Natural Products-Chemistry and Biological Significance, 1<sup>st</sup> ed. Longman group U. K. limited, Essex, 1994
2. I. L. Finar; Organic Chemistry, Vol. II, 5<sup>th</sup> ed. Pearson Education, 1956
3. M. Nogradi; Stereo selective synthesis- A Practical Approach, 2<sup>nd</sup> ed. Wiley-VCH, 1994
4. K. Hostettmann, M. P. Gupta and A. Marston; Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Harwood Academic Publishers, 1999

| Course Title/Code | Organic Laboratory (CHH 618B)   |
|-------------------|---|
| Course Type       | Core  |
| Course Nature     | Hard  |
| L-T-P-O Structure | 0-0-8-0   |
| Objectives        | To familiarize with synthesis of organic compounds<br>To familiarize with separation of organic compounds |
| Outcome           | The student will be able to understand isolation of natural products                                      |
| Prerequisites     | Organic Chemistry-I & II  |

#### LIST OF EXPERIMENTS

##### SEPARATION& ANALYSIS OF ORGANIC COMPOUNDS

1. Mixture of mannitol and p-toluidine
2. Mixture of glucose and cinnamic acid
3. Mixture of oxalic acid and m-dinitrobenzene or p-dinitrobenzene
4. Mixture of urea and acetanilide
5. Mixture of benzyl and p-toluidine
6. To prepare Hexamine cobalt (II) Chloride
7. To prepare Copper tetra iodide mercurate

8. To prepare Vanadylacetylacetonate

#### LIST OF EXPERIMENTS

##### TO SEPARATE AND ANALYSE THE ORGANIC COMPOUNDS

9. Mixture of benzoic acid and  $\beta$ -naphthol
10. Mixture of m-nitroaniline and hydroquinone
11. Mixture of tetrahydrofuran and cinnamic acid
12. Mixture of chloroform and benzidine
13. Mixture of aniline and benzamide
14. To prepare Chalcone (Benzene acetophenone)
15. To extract caffeine from tea leaves
16. To extract piperine from Black pepper
17. To prepare Dichlorodipyridinocobalt (II)
18. To prepare ammonium diamminetetraithiocyanato chromate (III)

#### Reference Books:

1. J. Singh, R. K. P. Singh, J. Singh, L. D. S. Yadav, I. R. Siddiqui and J. Srivastava; Advanced Practical Chemistry, 2<sup>nd</sup> ed. PragatiPrakashan, 2010
2. A. I. Vogel; Vogel's textbook of Practical Organic Chemistry, 5<sup>th</sup> ed. Longman Scientific and technical Publisher, UK, 1989
3. H. L. Fieser and F. L. Fieser, Organic Chemistry, Vol 1-11, Trade ed. 1944
4. B. M. Trost, I. Fleming and S. L. Scheiber; Comprehensive Organic Synthesis, 1<sup>st</sup> ed. Pergamon Press, 2007

|                          |  |
|--------------------------|--|
| <b>Course Title/Code</b> | <b>SCIENTIFIC RESEARCH-II (RDO603)</b>   |
| <b>Course Type</b>       | <b>Core</b>  |
| <b>L-T-P Structure</b>   | <b>0-0-8</b>   |
| <b>Credits</b>           | <b>4</b>   |
| <b>Course Objective</b>  | <b>To impart knowledge on various analytical techniques</b><br><b>To familiarize with the principle of analytical chemometrics</b> |

| Course Outcomes (COs) |  | Mapping           |
|-----------------------|--|-------------------|
| CO1                   | The students will be able to critically evaluate the work done by various researchers relevant to the research topic   | Skill Development |
| CO2                   | To integrate the relevant theory and practices followed in a logical way and draw appropriate conclusions  | Skill Development |
| CO3                   | To understand the research methodologies/approaches/techniques used in the literature  | Skill Development |
| CO4                   | To structure and organize the collected information or findings through an appropriate abstract, headings, reference citations and smooth transitions between sections | Skill Development |
| Prerequisites         | Scientific Research-I (RDO503)   |                   |

### SECTION A

#### Unit-1 Literature Survey (LS)/Design of Experiment

- 1.1 Collection of research papers related to previously identified gap/problem (15 papers or more)
- 1.2 Comprehend and arrange the literature based on the idea framed
- 1.3 Presenting the collected data and inferring it with the further scope of expansion and Designing the experiment wherever applicable.

### SECTION B

#### Unit-2 Structuring of Review Paper and setting up of experimental facility

- 2.1 Analysis of different approach/methodology adopted by various researchers
- 2.2 Listing out the components of the paper/ setting up experimental facility w.r.t the problem
- 2.3 Identification of suitable Journal or Conference
- 2.4 Formatting/Styling the paper according to the respective template

### SECTION C

#### Unit-3 Planning of experiments

- 3.1 Formulate experimental procedures with Modification of the experimental set-up, if required

### 3.2 Procurement of materials

#### **Unit-4 Execution of experiments/simulations**

4.1 Conduct experiments/ build prototype

4.2 Tabulating and recording data

4.3 Analysis and interpretation of the data

4.4 Comparison of the results with other reported experiments

4.5 Interpretation of observations

4.6 Integration of relevant theory, findings in a structured way and draw appropriate conclusions

### **SECTION D**

#### **Unit-5 Departmental Presentation**

5.1 Structuring and preparation of PPT

5.2 Mock presentation

5.3 Review on presentation skills and content delivered both

5.4 Incorporating the review comments in the slides

### **CO-PO Mapping**

| <b>Course Code</b> | <b>Course</b>                 | <b>Course Outcomes</b> | <b>PO1</b> | <b>PO2</b> | <b>PO3</b> | <b>PO4</b> | <b>PO5</b> | <b>PO6</b> | <b>PO7</b> | <b>PO8</b> | <b>PO9</b> | <b>PO10</b> | <b>PO11</b> |
|--------------------|-------------------------------|------------------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|-------------|
| <b>RDO603</b>      | <b>Scientific Research-II</b> | <b>CO1</b>             | -          | -          | -          | -          | -          | <b>3</b>   | <b>2</b>   | <b>3</b>   | -          | -           | -           |
|                    |                               | <b>CO2</b>             | -          | -          | -          | -          | -          | <b>2</b>   | <b>3</b>   | <b>3</b>   | -          | -           | -           |
|                    |                               | <b>CO3</b>             | -          | -          | -          | -          | -          | <b>3</b>   | <b>3</b>   | <b>2</b>   | -          | -           | -           |
|                    |                               | <b>CO4</b>             | -          | -          | -          | -          | -          | <b>3</b>   | <b>3</b>   | <b>3</b>   | -          | -           | -           |

# SEMESTER IV

(FOR ALL SPECIALIZATIONS)

|                   |                           |
|-------------------|---------------------------|
| Course Title/Code | Major Project (CHN 619 B) |
|-------------------|---------------------------|

|  |   |
|--|---|
| <b>Course Type</b>                               | Core  |
| <b>Course Nature</b><br><b>L-T-P-O Structure</b> | Hard<br>0-0-0-12  |
| <b>Objectives</b>                                | To impart understanding of research papers/articles in specific areas<br>To improve the communication skills by presentation on specific subjects<br>To improve the team work<br>To improve the research and practical approach |
| <b>Outcome</b>                                   | Student will be able to<br>Understand research and innovation skills<br>Enhance their communication skills<br>Start working in a team and improve their problem solving skills  |