

# **CHOICE BASED CREDIT SYSTEM (CBCS)**

**M. Sc.**

**Syllabus for Chemistry**



इन्दिरा गांधी राष्ट्रीय जनजातीय विश्वविद्यालय  
Indira Gandhi National Tribal University

अमरकंटक (म.प्र.) | Amarkantak (M.P.)

(भारतीय संसद में पारित अधिनियम द्वारा स्थापित केन्द्रीय विश्वविद्यालय)  
(A Central University Established by an Act of Parliament of India)

## ABOUT THE DEPARTMENT

### Department of Chemistry, IGNTU, Amarkantak

The Department of Chemistry was started in 2008, and has now grown into a major department for teaching and research within the Faculty of Science at IGNTU. The department offer vibrant atmosphere to students and faculty to encourage the spirit of scientific inquiry and to pursue cutting-edge research in a highly encouraging environment. The key objective of our department is to create good quality human resource through competitive yet inspiring environment for developing their careers. Currently, the department comprises more than hundred students, five research scholar and seven faculties and a dedicate team of staff members. The department offers three years undergraduate B.Sc. courses in Chemistry (Hons.) in the University. In addition it also offers two years M. Sc. and PhD programme. At present the Department consists of about seven research groups working in the areas of material chemistry (Functional Hybrid Nanomaterials), coordination/supramolecular chemistry, bioinorganic chemistry, asymmetric synthesis, catalysis, nanomagnetism and Single Molecule Magnets (SMMs), as major thrust areas. The department is doing well in research activities and published good numbers of research papers. The faculty has been undertaking research projects sponsored by different national agencies such as DST, UGC, etc. The most important achievement of the University is the first Department of Chemistry has succeeded “**DST-FIST Program – 2017**” recognition from Govt. of India, Department of Science & Technology, New Delhi. Many students have been qualified National Eligibility Test (NET) and Joint Admission Test (JAM) Examination for pursuing PhD and M. Sc. Program in different prestigious IIT, NIT and Central Universities. The most of the students of our department is tribal and our mission is that the department of Chemistry can be reached at highest level in the country for its teaching and research activities and produced number of best quality of students in India.

## At a Glance Department of Chemistry, IGNTU

### Faculty Profile

| Presentation  | Name & Designation   | Research Area  | Awards and Honors  |
|---|--|--|--|
|    | <b>Dr. Tanmay K Ghorai</b><br>Associate Professor & Head<br><i>PhD: IIT-KGP</i>  | Nanoscience, Catalysis & Single Molecule Magnets       | BOYSCAST Fellowship & Young Scientist Award (DST)            |
|    | <b>Dr. Subrata Jana</b><br>Associate Professor<br><i>PhD: IEST-Shibpur</i>       | Molecular Recognition & Supramolecular Chemistry       | Radhika Panda Memorial Award, UrFU PDF Award                 |
|   | <b>Dr. Khemchand Dewangan</b><br>Assistant Professor<br><i>PhD: IIT-Kanpur</i>   | Nanostructure Transition Metal Oxides & Nitrides       | BSR-UGC Start-Up Grant                                       |
|  | <b>Dr. Adhish Jaiswal</b><br>Assistant Professor<br><i>PhD: NCL-Pune</i>         | Dielectrics, Magnetism & Solar-cell                    | Best Research Scholar Award in NCL Pune                      |
|  | <b>Dr. Biswajit Maji</b><br>Assistant Professor<br><i>PhD: IIT-KGP</i>           | Asymmetric Synthesis and Catalysis                     | INSPIRE Faculty Award, President INSPIRE Teacher Recognition |
|  | <b>Dr. Sadhucharan Mallick</b><br>Assistant Professor<br><i>PhD: IITGuwahati</i> | Metal Particles, Polymer Composites & Bio applications | Best Poster Award at ICT Hyderabad                           |
|  | <b>Dr. Ajay Shankar</b><br>Assistant Professor<br><i>PhD: NPL, Delhi</i>         | Nano-magnetism   | Post-Doctoral fellowship Award at Germany                    |

**Members of the Board of Studies**

**For**

**Revised the Chemistry Syllabus for**

**M. Sc. Courses**

**According**

**CHOICE BASED CREDIT SYSTEM  
(CBCS)**

The syllabus of M.Sc. is hereby approved in a meeting of the members of the Board of Study for the Department of Chemistry, Indira Gandhi National Tribal University, Amarkantak (M.P.) on February 6, 2017, Monday.



**Prof. Ashish K. Prajapati**  
Professor  
(Member, External Expert)  
Department of Chemistry,  
The M. S. University of Baroda



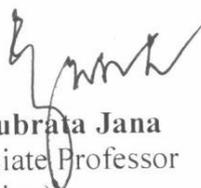
**Dr. Raghmani Singh Ningthoujam**  
Scientist-E  
(Member, Special Invitee)  
Chemistry Division  
Bhabha Atomic Research Centre



**Dr. Tarun Thakur**  
Associate Professor  
(Member)  
Department of Environmental Science  
IGNTU



**Dr. Ravindra Shukla**  
Assistant Professor  
(Member)  
Department of Botany  
IGNTU



**Dr. Subrata Jana**  
Associate Professor  
(Member)  
Department of Chemistry  
IGNTU



**Dr. Tanmay Kumar Ghorai**  
Associate Professor & Head  
(Chairman)  
Department of Chemistry  
IGNTU

| <b>Course Structure for M.Sc.</b>  |                         |   |               |
|--|-------------------------|---|---------------|
| <b>CHEMISTRY</b>   |                         |   |               |
| <i>1 credit = 1 hour per week for Theory and 2 hours per week for Laboratory</i> |                         |   |               |
| <b>Course Code</b>   | <b>Course Structure</b> | <b>Title of Paper</b>   | <b>Credit</b> |
| <b>SEMESTER-I</b>  |                         |   |               |
| CHM T 411  | Core                    | Catalysis-, Surface-, Electro- Chemistry & Chemical Kinetics  | 4             |
| CHM T 412  | Core                    | Transition and Inner Transition Metal Chemistry   | 4             |
| CHM T 413  | Core                    | Organic Reaction Mechanism and Stereochemistry  | 4             |
| CHM P 411  | Core                    | Inorganic Chemistry Practical - I   | 2             |
| CHM P 412  | Core                    | Organic Chemistry Practical - I   | 2             |
| GE/OE – I  |                         | Generic/Open Elective Course – I (any one course from elective section offered by Dept. of Chemistry)         | 3             |
| <b>SEMESTER-II</b>   |                         |   |               |
| CHM T 421  | Core                    | Quantum-, Statistical-Mechanics, Symmetry & Group Theory  | 4             |
| CHM T 422  | Core                    | Chemistry of Organometallics  | 4             |
| CHM T 423  | Core                    | Principle of Organic Synthesis and Organic Spectroscopy   | 4             |
| CHM P 421  | Core                    | Physical Chemistry Practical - I  | 2             |
| CHM P 422  | Core                    | Organic Chemistry Practical - II  | 2             |
| GE/OE – II   |                         | Generic/Open Elective Course – II (any one course from elective section offered by Dept. of Chemistry)        | 3             |
| <b>SEMESTER-III</b>  |                         |   |               |
| CHM T 511  | Core                    | Chemical Bonding, Non-equilibrium Thermodynamics and Solid State Chemistry                                    | 4             |
| CHM T 512  | Core                    | Bio-Inorganic & Nuclear Chemistry   | 4             |
| CHM T 513  | Core                    | Pericyclic Reaction, Photochemistry and Free Radical Chemistry  | 4             |
| DSE – I  |                         | Discipline Specific Elective Paper – I (any one course from elective section offered by Dept. Of Chemistry)   | 3             |
| CHM P 511  | Core                    | Physical Chemistry Practical – II   | 2             |
| CHM P 512  | Core                    | Inorganic Chemistry Practical – II  | 2             |
| <b>SEMESTER-IV</b>   |                         |   |               |
| CHM T 521  | Core                    | Molecular Spectroscopy  | 4             |
| DSE – II   |                         | Discipline Specific Elective Paper – II (any one course from elective section offered by Dept. Of Chemistry)  | 3             |
| DSE – III  |                         | Discipline Specific Elective Paper – III (any one course from elective section offered by Dept. Of Chemistry) | 3             |
| CHM P 522  | Core                    | Project and Dissertation  | 8             |
| <b>Grand Total (Semester I – IV)</b>   |                         |   | <b>75</b>     |

**GE: Generic Elective; OE: Open Elective; DSE: Discipline Specific Elective**

**\*Generic/Open Elective Course opted by the Other Department students**

## Elective Course

| Course Code | Course Structure | Title of Paper                                   | Credit |
|-------------|------------------|--|--------|
| CHM T 601   | Elective         | Mathematics for Chemist                          | 3      |
| CHMT 602    | Elective         | Biology for Chemist                              | 3      |
| CHM T 603   | Elective         | Industrial Chemistry                             | 3      |
| CHM T 604   | Elective         | Instrumental Methods of Analysis                 | 3      |
| CHM T 605   | Elective         | Basic of Materials Chemistry                     | 3      |
| CHM T 606   | Elective         | Introduction to Nanomaterials and Nanotechnology | 3      |
| CHM T 607   | Elective         | Polymers Chemistry                               | 3      |
| CHM T 608   | Elective         | Bioorganic and Drug Chemistry                    | 3      |
| CHM T 609   | Elective         | Advanced Heterocyclic Chemistry                  | 3      |
| CHM T 610   | Elective         | Chemistry of Natural Products                    | 3      |
| CHM T 611   | Elective         | Solid State Chemistry                            | 3      |
| CHM T 612   | Elective         | Advanced Synthetic Organic Chemistry             | 3      |

## SEMESTER – I

### CHM T 411: Catalysis-, Surface-, Electro- Chemistry & Chemical Kinetics

Credits: Theory-04

Theory: 60 Hours

#### Unit – 1: Heterogeneous Catalysis

**Heterogeneous Catalysis (Surface Reactions):** Kinetics of uni-molecular reactions-inhibition and activation energy. Bimolecular surface reactions - reactions between a gas molecule and an adsorbed molecule, reaction between two adsorbed molecules. Effect of temperature on surface reaction promoters and poisons.

(10 Hours)

#### Unit – 2: Homogeneous Catalysis

**Kinetics Homogeneous Catalysis:** Nature of surface, concept of active centers. Kinetics of enzymatic reactions: Michaelis-Menten equation, Lineweaver-Burk and Eadie Analyses, enzyme inhibition (competitive, non-competitive and uncompetitive inhibition), effect of temperature and pH of enzymatic reaction; acid – base catalysis and their mechanism.

(10 Hours)

#### Unit – 3: Electrochemistry

**Electrochemistry of Solution:** Debye-Hückel treatment for mean ionic activity coefficient and its extension, ion solvent interaction and Debye-Hückel-Baerrum model. Thermodynamic of electrified interfaces, electrocapillary measurement of interfacial tension, derivations Lippmann equation (surface excess) and determination of surface excess. Structure of electrified interfaces, Helmholtz-Perrin, Gouy-Chapmann, Stern models, Graham-Devanathan Mottwatts, Tobin, Bockris, Devanathan Models.

**Over Potential:** Exchange current density, derivation of Butler-Volmer equation, Tafel plot. Quantum aspect of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling.

**Corrosion:** Introduction to corrosion, homogeneous theory, forms of corrosion, corrosion monitoring and prevention method.

(12 Hours)

#### Unit – 4: Surface Chemistry

**Surface Tension:** Capillary action, pressure difference across curved surface (Laplace equation), vapor pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface film and liquids (electro-kinetic phenomenon), catalytic activities at surface.

**Surface Active Agents:** Classification of surface active agents. Micellization, hydrophobic interaction, critical micellar concentration (CMC), factor affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro-emulsion reverse micelles.

(12 Hours)

#### Unit – 5: Chemical Kinetics

Rate law, method of determining rate laws, General feature of fast reactions, study of fast reaction by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method.

**Reactions in Gas Phase:** Theories of Reaction Rates- Arrhenius theory, collision theory and transition state theory, potential energy surface, enthalpy, free energy and entropy of activation, correlation of steric factor in collision theory and entropy of activation (Thermodynamic parameter). Uni-molecular reactions: Lindeman-Hinshelwood theory, Rice-Ramsperger-Kassel (RRK) theory, Rice- Ramsperger-Kassel- Marcus(RRKM) theory.

**Elementary Reactions in Solution:** Comparison between gas-phase and solution-phase reactions, factor determining reaction rates in solution; ionic reaction [influence of solvent, influence of ionic strength (salt effect)] ; Linear Free Energy Relationships, (LFER), Effect of substituent on reaction rates (Hammett relationships). Kinetics of isotopic effect.

**Dynamic of Molecular Motion:** probing the transition state, dynamics of barrier-less chemical reaction in solution.

**Chain Dynamic:** (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reaction), and Oscillatory reaction, autocatalysis (Belousov-Zhabotinsky reaction).

(16 Hours)

#### Reference Books:

- K. J. Laidler, *Chemical Kinetics*, Eds: 3<sup>rd</sup>, Pearson, 2011.
- J. Rajaram and J. C. Kuriacose: *Kinetics and Mechanisms of Chemical Transformations Applications of Femto-chemistry*, MacMillan, New Delhi, 2011.
- B. R. Puri, L. R. Sharma and M. S. Pathania: *Principle of Physical Chemistry*, Eds. 44<sup>th</sup>, Vishal Publishing Co., Jalandhar, 2010.
- P. Atkins and J. D. Paula: *Physical Chemistry*, Eds. 7<sup>th</sup>, Oxford University Press, New Delhi, 2002.
- R. S. Berry, S. A. Rice and J. Ross: *Physical Chemistry*, Eds: 2<sup>nd</sup>, Oxford University Press, New Delhi, 2007.
- J. O'M Bockris, A. K. N. Reddy and M. Gamboa-Aldeco: *Modern Electrochemistry Vol-1 and Vol-2*, Springer, 2006.
- D. R. Crow: *Principles and Applications of Electrochemistry*, Eds. 4<sup>th</sup>, Blackie Academic & Professional, Madras, 1994.
- V. S. Bagotsky: *Fundamental of Electrochemistry*, Wiley-Interscience, 2006.

# CHM T 412: Transition and Inner Transition Metal Chemistry

Credits: Theory-04

Theory: 60 Hours

## Unit – 1: Coordination Chemistry

Experimental evidence of metal-ligand overlap, spin orbit coupling constant and interelectronic coupling parameters in complex ion terms-vs-free ion terms, Nephelauxetic effect,  $d$ -orbital splitting in octahedral, Jahn-Teller distorted octahedral, square planar, square pyramidal, trigonal bipyramidal, and tetrahedral complexes, CFSE for  $d^1$  to  $d^{10}$  systems, pairing energy, low-spin and high-spin complexes and magnetic properties, Crystal field activation energy, hole formalism, Tetrahedral distortion and Jahn Teller effect, Static and Dynamic Jahn-Teller effect, Effect of crystal field stabilization on ionic radii, lattice energy, hydration enthalpy and stabilization of complexes (Irving Williams order). Colour and spectra, Kinetic aspects of crystal field stabilization. adjusted CFT, Limitations of CFT, Labile and inert complexes.

(12 Hours)

## Unit – 2: Electronic Spectra of Transition Metal Complexes

Microstates, Russell-sander's terms, determination of ground and excited state terms of  $d^n$  ions; Orgel diagrams (qualitative approach) and Tanabe-Sugano diagram, selection rules for spectral transitions,  $d-d$  spectra of  $d^n$  ions and crystal field parameters, nephelauxetic series, Electronic Spectra UV-Vis, charge transfer, colors, intensities and origin of spectra. MOT to rationalize  $\sigma$  and  $\pi$  interactions in octahedral, square planar and tetrahedral metal complexes. Symmetry designations of LGOs and MOs. Simplified MO diagrams.

(12 Hours)

## Unit – 3: Magneto Chemistry

Basic principles of magnetism, Magnetic properties, paramagnetism, ferro- and antiferro magnetism, diamagnetism, Pascal constants, Currie equation, determination of magnetic susceptibility, application of Van Vleck susceptibility equation, Magnetic properties and coordination compounds Spin and orbital moments, spin – orbit coupling, quenching of orbital moment, spin only formula, room temperature and variable temperature magnetic moments and spin crossover. Magnetic properties of first transition series metal ions, lanthanides and actinides, Lanthanide and actinide contractions and their consequences, separation of lanthanides and actinides and their applications (examples). magnetic exchange interactions. ESR spectroscopy, Basic concept of Single Molecule Magnets (SMM), properties, examples and application of SMMs.

(12 Hours)

## Unit – 4: Inorganic Reaction Mechanism

Mechanism of substitution reactions, solvent exchange, aquation, anation, base hydrolysis, acid catalyzed aquation, pseudo-substitution. Energy profile diagram of ligand substitution reactions- associative (A), dissociative (D), interchange (I) etc. type pathways, relation between intimate and stoichiometric mechanisms of ligand substitution, some important rate laws, activation parameters ( $\Delta S^\ddagger$ ,  $\Delta H^\ddagger$ ,  $\Delta V^\ddagger$ ), mechanism of isomerization reaction-linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racimization, Ray-Dutta and Bailar twist mechanisms, substitution in octahedral complexes- the Eigen-Wilkins mechanism, the Fuoss-Eigen equation, linear free energy relation (LFER) etc. Mechanism of

electron transfer reactions: General characteristics and classification of redox reactions, self-exchange reactions. Frank-condon principle (non mathematical treatment). Outer sphere and Inner sphere reactions, applications of Marcus expression (simple form), redox catalyzed substitution reactions.

(12 Hours)

### Unit - 5: Chemistry of Elements

**d-Block Elements:** Electronic configuration, oxidation states; aqueous, redox and coordination chemistry, spectral and magnetic properties of compounds in different oxidation states, horizontal and vertical trends in respect of 3d, 4d, and 5d elements with references to Ti-Zr- Hf , V-Nb-Ta, Cr- Mo- W, Mn-Tc-Re and Pt group metals. Occurrence and isolation in respect of V, Mo, W, Re, Pt. Iso- and heteropolyoxometalates with respect to V, Mo, and W: synthesis, reactions, structures, uses, metal-metal bonded dinuclear d-metal complexes (examples), Bonding in dirhenium complexes.

### Qualitative Analysis of Inorganic Radicals

Introduction to salt analysis, dry and wet test for acid and basic radicals, Principle and chemistry of qualitative analysis of inorganic salt; chemistry involved in qualitative analysis of mixture containing interfering radicals and insolubles.

(12 Lectures)

### Reference Books:

- J. D. Lee: *A new Concise Inorganic Chemistry*, E L. B. S.
- D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
- Douglas, McDaniel and Alexander: *Concepts and Models in Inorganic Chemistry*, John Wiley.
- B. R. Puri, L. R. Sharma, and K. C. Kalia: *Principle of Inorganic Chemistry*, Milestone Publisher, New Delhi 2010.
- W. U. Malik, G. D. Tuli, and R. D. Madan: *Selected Topic in Inorganic Chemistry*, S. Chand & Company Ltd, New Delhi, 1998.
- J. E. Huheey, E. A. Keiter, R. L. Keiter, and O. K. Medhi: *Inorganic Chemistry Principle of Structure and Reactivity*, Eds: 4<sup>th</sup> Pearson, New Delhi, 2006.
- F. A Cotton, G. Wilkinson, C. A. Murillo, and M. Bochmann: *Advanced Inorganic Chemistry*, Eds: 6<sup>th</sup>, Wiley-India, New Delhi, 2010.

# CHM T 413: Organic Reaction Mechanism and Stereochemistry

Credits: Theory-04

Theory: 60 Hours

## Unit – 1: Physical Organic Chemistry

- (i) Thermodynamic and kinetic requirements of a reaction: Transition state theory, Hammond's postulate, Kinetic vs Thermodynamic control
- (ii) Acids and Bases
- (iii) Determining the mechanism of a reaction: Detection and trapping of intermediates, Cross-over experiments, kinetic isotopic effect-primary kinetic and secondary kinetic isotopic effect

(12 Hours)

## Unit – 2: Substitution, Addition, and Elimination Reactions

**Substitution Reaction:** Aliphatic nucleophilic substitution-  $S_N1$ ,  $S_N2$ ,  $S_{Ni}$  mechanism, classical and nonclassical carbocations, phenonium ions, NGP-in substitution reactions. Effect of solvent, structure, nucleophile and leaving group on rate of  $S_N1$ , and  $S_N2$  reaction. Electrophilic aromatic substitution and Nucleophilic aromatic substitutions. Mechanism and stereo chemical aspects of substitution reactions.

**Addition Reaction:** Addition to carbon-carbon multiple bonds, addition to carbon-heteroatom multiple bonds, electrophilic, nucleophilic and free radical addition reactions. Mechanism and stereo chemical aspects of addition reactions.

**Elimination Reaction:**  $E1$ ,  $E2$ ,  $E1c_b$  mechanisms, orientation and stereochemistry in elimination reaction, reactivity effect of structure, attacking and leaving group, competition between elimination and substitution, syn-eliminations.

(14 Hours)

## Unit – 3: Symmetry Operation and Stereoisomerism

Simple or proper axis of symmetry, plane of symmetry, centre of symmetry and improper or rotation-reflection of symmetry. Enantiomerism and diastereomerism, conventions for configurations D-L and R-S systems, Threo and erythro nomenclature. Measurement of optical purity, enantiomeric excess. Stereoselective and Stereospecific reactions. Molecules with tri- and tetra coordinated chiral centres. Molecules with two or more chiral centres.

(12 Hours)

## Unit – 4: Chirality and Conformations

**Axial and Planar Chirality:** Principles of axial and planar chirality. Stereochemistry of allenes, Stereochemistry of biphenyl derivatives and atropisomers. Stereochemistry of spiranes, Stereochemistry of molecules with planar chirality, Helicity.

**Conformations & Stereoisomerism of Acyclic and Cyclic Systems:** Molecular mechanics and conformations, Conformations of a few acyclic molecules, Conformations of cyclic systems: monocyclic compounds (mono, di- and poly substituted cyclohexanes); Conformations of fused ring and bridged ring compounds.

(10 Hours)

## Unit – 5: Dynamic Stereochemistry

**Conformation and Reactivity:** Conformation, reactivity and mechanism: Cyclic systems (Nucleophilic substitution reaction at ring carbon, Addition reaction to double bonds, Elimination reactions, NGP reactions). Conformation, reactivity and mechanism: Acyclic systems (addition, Elimination and NGP participation). Formation and reaction of enols and enolates. Reduction of cyclohexanes with hydride reagents.

**Stereoselective Reactions:** Principle of stereoselectivity, asymmetric synthesis and asymmetric induction, Acyclic stereoselections (addition of nucleophiles to carbonyl compounds, aldol reactions, addition to allyl metal and allyl boron compound to carbonyl compounds), Diastereoselections in cyclic systems (Nucleophilic addition to cyclic ketones, alkylations, catalytic hydrogenations).

**(12 Hours)**

**Reference Books:**

- J. Clayden, N. Greeves, S. Warren and P. Wothers: *Organic Chemistry*, Oxford
- J. March: *Advanced Organic Chemistry*, 6th Edition
- A. Carey and R.J. Sundberg: *Advance Organic Chemistry* (part A)
- Paula Y Bruice: *Organic Chemistry*
- E.L. Eliel: *Stereochemistry of carbon compound*
- Nasipuri: *Stereochemistry of organic compound*
- Peter Sykes: *Guide book to Reaction Mechanism*

## CHM P 411: Inorganic Chemistry Practical – I

Credits: 02

Lab: 60 Hours

### A. Qualitative Analysis

Semi-micro qualitative analysis of mixture containing eight radicals including two less common metal from among the following:

(1) **Basic Radicals:**  $\text{Ag}^+$ ,  $\text{Pb}^{2+}$ ,  $\text{Bi}^{3+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{As}^{3+}$ ,  $\text{Sb}^{3+}$ ,  $\text{Sn}^{4+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Al}^{3+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Ce}^{3+}$ ,  $\text{Th}^{4+}$ ,  $\text{Zr}^{4+}$ ,  $\text{W}^{6+}$ ,  $\text{Te}^{4+}$ ,  $\text{Ti}^{4+}$ ,  $\text{Mo}^{6+}$ ,  $\text{V}^{5+}$ ,  $\text{Be}^{2+}$ .

(2) **Acid Radicals :** Carbonate, Sulphite, Sulphide, Nitrite, Nitrate, Acetate, Fluoride, Chloride, Bromide, Iodide, Sulphate, Borate, Oxalate, Phosphate, Silicate, Thiosulphate, Ferrocyanide, Ferricyanide, Thiocyanide, Chromate, Arsenate and Permanganate.

### B. Chromatographic Separation

- Use paper chromatography to separate and identify the metal ion components of an unknown solution.
- Chromatographic separation of sugars, amino acids by paper, T.L.C. and Ion exchange.

### C. Standard Deviation

- Calculation of standard deviation from the results obtained by redox titration of Fe(III) against standard solution of  $\text{K}_2\text{Cr}_2\text{O}_7$ .
- Calculation of standard deviation from the results obtained by complexometry method of hardness ( $\text{Ca}^{2+}$ ) of water using EDTA.

### Reference Books:

- A.I. Vogel: *Qualitative Inorganic Analysis*, Prentice Hall, 7th Edn.
- A.I. Vogel: *Quantitative Chemical Analysis*, Prentice Hall, 6th Edn.
- B.D. Khosla: *Senior Practical Physical Chemistry*, R. Chand & Co.
- P. C. Comboj: *University Practical Chemistry*, Vishal Publishing Co. Jalandhar.

## CHM P 412: Organic Chemistry Practical – I

Credits: 02  
Lab: 60 Hours

### Part A: Techniques of Separation and Purification

- Fractional Distillation of a mixture of liquids
- Distillation under reduced pressure
- Chromatographic separation (Paper chromatography and Thin Layer Chromatography)

### Part B: Analysis of Organic Binary Mixture

- Separation and Identification of organic compounds from the given binary mixtures. (Complete study of determination of organic compound with melting point and preparation of a suitable derivative)

### Part C: Preparation of Organic Compounds (Single Stage Preparation)

Representative reactions to be covered:

- Electrophilic aromatic substitution reaction (Friedel-Crafts Reaction, halogenation, nitration and sulphonation reaction)
- Acetylation reaction
- Diels-Alder reaction
- Condensation reaction
- Cannizzaro reaction
- Oxidation reaction
- Reduction reaction
- Rearrangement reaction
- Esterification
- Diazotization reaction
- Sandmeyer reaction

### Reference Books:

- A. I. Vogel: *Practical Organic Chemistry*
- F. G. Mann and B. C. Saunders: *Practical Organic Chemistry*
- J. Leonard, B. Lygo and G. Proctor: *Advanced Practical Organic Chemistry*.
- Addison Ault: *Techniques and Experiments for Organic Chemistry*, University Science Book
- R. L. Shriner and D. Y. Curtin: *The Systematic Identification of Organic Compounds*
- B. S. Roa and V. Deshpande: *Experimental Biochemistry*, I. K. Pvt. Ltd.
- V. K. Ahluwalia and Renu Aggarwal: *Comprehensive Practical Organic Chemistry, Preparation and Qualitative Analysis*
- Ghoshal, Mahapatra and Nad: *An Advanced Course in Practical Chemistry*.

## SEMESTER – II

### CHM T 421: Quantum-, Statistical- Mechanics, Symmetry & Group Theory

Credits: Theory-04

Theory: 60 Hours

#### Unit – 1: Quantum Chemistry – I

**Historic Background:** Important historic background of quantum mechanics versus classical mechanics, wave particle duality, Heisenberg's uncertainty principle.

**Schrödinger Wave Equation:** normalization and orthogonality of wave functions; time-dependent and time-independent Schrödinger equations.

**Operators:** Operators and their algebra, linear and Hermitian operators, matrix representation, commutation relationship, quantum mechanical operators for position, linear momentum, angular momentum, total energy, eigenfunctions, eigenvalues and eigenvalue equation; expansion of arbitrary state in term of complete set, postulates of quantum mechanics.

**Solution of the Schrödinger Equations for Some Exactly Soluble Systems:** particle-in-a-box; particle-in-a-ring and -sphere; harmonic oscillator; tunneling one dimensional potential barrier and well.

(12 Hours)

#### Unit – 2: Quantum Chemistry – II

**Rigid Rotor,** spherical coordinates Schrödinger wave equation in spherical coordinates, separation of the variables, the  $\phi$  equation, wave-function, quantum number, the  $\theta$  equation, wave function, quantization of rotational energy, spherical harmonics.

**Hydrogen and Hydrogen Like Atoms:** Radial and angular probability distributions, atomic orbitals.

**Angular Momentum:** Basis functions and representation of orbital angular momentum operators, eigenfunctions, and eigenvalues of orbital angular momentum operator, Ladder operator, Spin, spin angular momenta, coupling (orbital and spin) of angular momentum, Clebsch-Gordan coefficients and Wigner Eckart theorem.

**Approximate Methods of Quantum Mechanics:** Variational principle; time-independent perturbation theory up to second order in energy for non-degenerate and degenerate system with simple examples; application to the two electron system such as, He and He like atoms.

(12 Hours)

#### Unit – 3: Atomic Structure and Spectroscopic

Many electron atoms, Pauli antisymmetry principle, Hund's rules; Slater determinant; Hartree and Hartree-Fock self consistent field model for atom; electronic term symbol (Russell-Saunders and jj coupling) for atoms and spectroscopic states (selection rules for atomic spectra).

(12 Hours)

#### Unit – 4: Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging; conical, grand conical and micro-canonical ensembles. Boltzmann distribution laws (using Lagrange's method of undetermined multipliers). Partition function – translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in term of partition function, Applications of partition functions.

Heat capacity behavior of solid – chemical equilibria and equilibrium constant in term of partition function. Fermi-Dirac statistics, distribution law and application to metal, Bose-Einstein statistics, distribution law and application to helium.

**(12 Hours)**

### **Unit – 5: Symmetry & Group Theory**

Symmetry elements and symmetry operations; point groups, Schoenflies notation for point group, representation of group by matrix, character of a representation, reducible and irreducible representation, great orthogonality theorem and its importance.

Application of group theory to atomic orbitals in ligand fields, molecular orbitals, and hybridization. Selection rules for IR and Raman spectra, procedure for determining symmetry of normal modes of vibration - hybrid orbitals in  $\text{BF}_3$ ,  $\text{CH}_4$ ,  $\text{NH}_3$ ,  $\text{H}_2\text{O}$  and  $\text{SF}_6$ .

**(12 Hours)**

### **Reference Books:**

- Ira. N. Levine: *Quantum Chemistry*, Eds: 5<sup>th</sup>, PHI, 2000.
- A. K. Chandra: *Introductory Quantum Chemistry*, Eds: 4<sup>th</sup>, Tata McGraw Hill, New Delhi, 1994.
- P. Atkins and R. Friedman: *Molecular Quantum Mechanics*, Eds: 5<sup>th</sup>, Oxford University Press, 2011.
- T. Engle and P. Reid: *Quantum Chemistry and Spectroscopy*, Pearson, New Delhi, 2011.
- B. Widom: *Statistical Mechanics: A Concise Introduction for Chemist*, Cambridge University Press.
- K. J. Laidler, *Chemical Kinetics*, Eds: 3<sup>rd</sup>, Pearson, 2011.
- F. A. Cotton, *Symmetry & Group Theory*.

# CHM T 422: Chemistry of Organometallics

**Credits: Theory-04**

**Theory: 60 Hours**

## Unit – 1: Organometallics – I

Organo transition metal chemistry: History, Nature of metal – carbon bonding and definition and classification of organometallic compounds, classification ligands, kinetic and thermodynamic stability of organometallic compounds. Compounds with metal carbon  $\sigma$  and multiple bond: Heptacity complexes of Metal-alkyl, -allyl, aryl, -carbene (Fischer and Schrock type), -carbonyl, -carbinos and cyclopentadienyl complexes Synthesis, bonding, stability, reactivity and decomposition pathway, Reactions in organometallic compounds. Structure and bonding in  $\eta^2$ -ethylenic and  $\eta^3$ -allylic compounds with typical examples, structure and bonding of  $K[Pt(C_2H_4)Cl_3]$ ,  $[(Ph_3P)_2Pt(Ph-C\equiv C-Ph)]$ . Fluxional organometallic compounds: Fluxionality and dynamic equilibria in compounds such as  $\eta^2$  olefins,  $\eta^3$  allyl and diene complexes, techniques of study.

**(12 Hours)**

## Unit – 2: Organometallics – II

Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

Catalysis by organometallic compounds: Hydrogenation of olefins, Wilkinson's catalyst, Tolman catalytic loop; synthesis gas, water-gas shift reaction; Hydroformylation (oxo process), Monsanto acetic acid process, Wacker process; synthetic gasoline: Fischer-Tropsch process and Mobile process, polymerization, oligomerization and metathesis reactions of alkenes and alkynes, Ziegler-Natta catalysis, photo dehydrogenation catalyst (platinum POP).

**(12 Hours)**

## Unit – 3: Inorganic Rings, Cages and Clusters

Polymorphism of C, P and S. Structure and bonding in higher boranes and borohydrides-Lipscomb's topological models, Wade's rules, carboranes and metallocenecarboranes.

Metal-metal bonding (M.O. Approach), metal-metal single and multiple bonded compounds. Low nuclearity ( $M_3$ ,  $M_4$ ) and high nuclearity ( $M_5$ - $M_{10}$ ) carbonyl clusters: skeletal electron counting, Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, Nb and Ta clusters, Mo and W clusters. Cluster compounds in catalysis.

**(12 Hours)**

## Unit – 4: New Developments in Organometallics Chemistry Research

Construction, structure and property of compounds with specific topology in Organometallic Chemistry: Capsules, boxes, containers, prisms or clusters, tubes, catenanes, rotaxanes,

incorporation of metal atoms through metal-ligand coordination interactions, Various organic ligands containing carboxy, imidazole or pyridine groups, which can coordinate with metal atoms, have been used to generate the desired compounds (V, Cr, Mn, Fe, Co, Ni, Cu). Particularly, flexible ligands with central aromatic core and imidazol-1-ylmethyl pendant arms, e.g. 1,3,5-tris(imidazol-1-ylmethyl)-2,4,6-trimethylbenzene and its analogues, Interesting properties: olecular recognition, ion inclusion and exchange of these compounds, especially of the cage-like compounds, are described.

(12 Hours)

#### Unit – 5: Metal – ligand equilibria in solution

Stability of mononuclear, polynuclear and mixed ligand complexes in solution. Stepwise and overall formation constants and their relations. Trends in stepwise formation constants, factors affecting the stability of metal complexes with reference to the nature of the metal ions and ligands. Statistical and non-statistical factors influencing stability of complexes in solution. Stability and reactivity of mixed ligand complexes with reference to chelate effect and thermodynamic considerations. Macrocyclic and template effect. Spectrophotometric and pH metric determination of binary formation constants.

(12 Hours)

#### Reference Books:

- J. E. Huheey, E. A. Keiter, R. L. Keiter, and O. K. Medhi: *Inorganic Chemistry Principle of Structure and Reactivity*, Eds: 4<sup>th</sup> Pearson, New Delhi, 2006.
- F. A Cotton, G. Wilkinson, C. A. Murillo, and M. Bochmann: *Advanced Inorganic Chemistry*, Eds: 6<sup>th</sup>, Wiley-India, New Delhi, 2010.
- D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
- Douglas, McDaniel and Alexander: *Concepts and Models in Inorganic Chemistry*, John Wiley.
- Robert Crabtree: *The Organometallic Chemistry of the Transition Metals*, 3rd Edition, Wiley.
- Collman, Hegedus, Norton and Finke: *The Principles and Applications of Transition Metal Chemistry*, 2nd Eds, University Science Books.
- Christoph Elschenbroich: *Organometallics*, 3rd Edition,
- Wei-Yin Sun, *New Developments in Organometallics Chemistry*, Wiley

# CHM T 423: Principle of Organic Synthesis and Organic Spectroscopy

Credits: Theory-04

Theory: 60 Hours

## Unit – 1: Principles of Organic Synthesis

**Acid Catalyzed Carbon-Carbon Bond Formation Reaction:** Principles, Self condensation of alkenes, reactions of aldehydes and ketones, Friedel-Crafts reactions, Prins reaction and Mannich reaction and Nef Reaction.

**Base Catalyzed Reactions (Enolate Chemistry):** Enolates: structure and stability of enolates, Generation of enolates using Nucleophilic and non Nucleophilic bases. Kinetic and Thermodynamic control of regioselectivity of enolates, Reactions of enolates. Alkylation and acylation of enolates: Haloform reaction, HVZ reaction, Claisen condensation, Enolate of active methylene compounds and corresponding alkylation reactions, Michael addition, Robinson annulations reaction.

(12 Hours)

## Unit – 2: Rearrangement and Organometallic Reactions

**Rearrangement Reactions:** Demjanov, Pummerer, Dienone-phenol rearrangement, Pinacol-Pinacolone rearrangement, Fries rearrangement, Wagner-Meerwein Rearrangement, Benzil-Benzilic Acid Rearrangement, Beckmann Reaction, Curtius, Schmidt, Lossen, Hoffman and Claisen rearrangement. Brook, Favorski, Neber, Von Richter, Sommelet Hauser and Wittig rearrangement.

**Organometallic Reagents:** Organomagnesium and Lithium reagents (Preparations, uses and applications), uses of Organomercury, organocadmium, organozinc and organocopper compounds.

(12 Hours)

## Unit – 3: Ultraviolet and Infrared Spectroscopy

**Ultraviolet Spectroscopy:** Factors affecting the position and intensity of UV bands – effect of conjugation, steric factor, pH, solvent polarity. Calculation of absorption maxima by Woodward-Fieser Rules (using Woodward-Fieser tables for values for substituent's) for the following classes of organic compounds: conjugated polyenes (cyclic and acyclic), enones and substituted benzene derivatives.

**Infrared Spectroscopy:** Fundamental, overtone and combination bands, vibrational coupling, important group frequencies for the common functional groups.

## Unit – 4: Nuclear Magnetic Resonance and Mass Spectroscopy

**Nuclear Magnetic Resonance Spectroscopy:** Chemical shift, Factors affecting chemical shift, Chemical and magnetic equivalence, Spin-spin coupling, Coupling constant J, Factors affecting J, Karplus equation, First order spectra, Geminal, vicinal and long range coupling (allylic and aromatic). <sup>13</sup>C NMR, Heteronuclear coupling, 2D NMR spectroscopy.

**Mass Spectrometry:** Molecular ion peak, base peak, isotopic abundance, metastable ions. Nitrogen rule, Determination of molecular formula of organic compounds based on isotopic abundance and HRMS Fragmentation pattern in various classes of organic compounds (including compounds containing hetero atoms), McLafferty rearrangement, Retro-Diels-Alder reaction, ortho effect.

(14 Hours)

## Unit – 5: Structure Determination of Organic Compounds

Structure determination involving individual or combined use of the above spectral techniques.

(10 Hours)

### Reference Books:

- J. Clayden, N. Greeves, S. Warren and P. Wothers: *Organic Chemistry*, Oxford
- A. Carey and R.J. Sundberg: *Advance Organic Chemistry (Part B)*.
- Parikh, Parikh and Parikh: *Name reactions in Organic Synthesis*, Foundation Books, 2006.
- G. Brahmachari: *Organic Name Reactions*, Narosa Publishers, 2009.
- J. J. Li: *Name reactions in organic synthesis*, 3<sup>rd</sup> Edition, SPRINGER 2006.
- Bessler and Silverstein: *Spectroscopy of Organic Compounds*, JOHN WILEY, 2001.
- D. C. Pavia, G. M. Lampman, G. S. Kriz: *Introduction to Spectroscopy*, 3<sup>rd</sup> Edition, Thomson, 2007.
- William Kemp: *Organic Spectroscopy*, III Edition

## CHM P 421: Physical Chemistry Practical – I

**Credits: 02**  
**Lab: 60 Hours**

- (i) Chemical Kinetics
  - (a) Kinetics of Reaction between ferric nitrate and potassium iodide using initial reaction rates.
  - (b) Determination of the rate constant for the decomposition of hydrogen peroxide by  $\text{Fe}^{3+}$  and  $\text{Cu}^{2+}$  ions.
  - (c) Flowing clock reactions (Experiments in physical Chemistry by Shoemaker).
- (ii) Determination of CMC of the surfactant/CMC Concentration.
- (iii) Determination of partial molal volume.
- (iv) Determination of the isotherm for a three component system.
- (v)
  - (a) Spectrophotometric determination of acid dissociation constant.
  - (b) Formula and stability constant using spectrophotometry.

### Reference Books:

- A. M. James and F. E. Prichard: *Practical Physical Chemistry*, Longman.
- B. P. Levi: *Findley's Practical Physical Chemistry*,
- R. C. Das and B. Behera: *Experimental Physical Chemistry*, Tata McGraw Hill.
- D. P. Shoemaker, G. W. Garland and J. W. Niber: *Experimental Physical chemistry*, Mc Graw Hill Interscience.
- A. J. Elias: *A collection of Interesting General Chemistry Experiments*, University Press, India.
- J. Rose: *Advanced Physico-Chemical Experiments*, Sir Isaac Pitman & Sons Ltd, London.
- J. B. Yadav: *Advanced Practical Physical Chemistry*, Krishna Prakashan Media (P) Ltd. Meerut.
- P. C. Comboj: *University Practical Chemistry*, Vishal Publishing Co. Jalandhar.

## CHM P 422: Organic Chemistry Practical – II

Credits: 02

Lab: 60 Hours

### Part A: Multi Step Synthesis of Organic Compounds

Multi step organic synthesis involving the concept of protecting groups and selectivity in organic reaction. A Student must be involved to check TLC for monitoring the reaction progress and doing column chromatography for purification.

Characterization of synthesized organic compounds using IR, UV and NMR, and mass spectroscopic techniques are to be studied.

- Nitrobenzene → aniline → Acetanilide (Nitration and followed by reduction)
- Malonic acid → cinnamic acid → methyl cinnamate (Condensation reaction and next followed by esterification)
- Benzaldehyde → benzoin → benzil → benzilic acid (Umpolung strategy, Oxidation reaction and next benzylic acid rearrangement reaction)
- Aniline → benzenediazonium chloride → benzeneazo-2-naphthol (Azodye synthesis)
- Skraup's synthesis: Quinoline from *o*-aminophenol (Heterocyclic compound synthesis)
- Acetanilide → *p*-acetamidobenzenesulfonylchloride → *p*-acetamidobenzenesulfonamide → sulfanilamide (Sulfa Drug synthesis)
- cinnamaldehyde → cinnamyl alcohol → cinnamyl bromide → allyl-aryl ether synthesis (Nucleophilic substitution reaction)

### Part B: Extraction Method

- **Natural product extraction:** Solasidine, Caffeine, Nicotine, Peptine, Rosine, Carotenoids, Computational methods of retro-synthetic analysis modeling and calculation.

### Reference Books:

- A. I. Vogel: *Practical Organic Chemistry*
- F. G. Mann and B. C. Saunders: *Practical Organic Chemistry*
- J. Leonard, B. Lygo and G. Proctor: *Advanced Practical Organic Chemistry*
- Addison Ault; *Techniques and Experiments for Organic Chemistry*, University Science Book
- R. L. Shriner and D. Y. Curtin: *The Systematic Identification of Organic Compounds*
- B. S. Roa and V. Deshpande: *Experimental Biochemistry*, I. K. Pvt. Ltd.
- V. K. Ahluwalia and Renu Aggarwal: *Comprehensive Practical Organic Chemistry, Preparation and Qualitative Analysis*
- Nad, Mahapatra and Ghoshal: *An Advanced Course in Practical Chemistry*

## SEMESTER – III

### CHM T 511: Chemical Bonding, Non-equilibrium Thermodynamics and Solid State Chemistry

Credits: Theory-04  
Theory: 60 Hours

#### Unit – 1: Molecular Structure

Chemical bonding in diatomic; elementary concepts of MO and VB theories; Born-Oppenheimer approximation, MO treatment for  $H_2^+$  ion, MO treatment of homo- and hetero-nuclear diatomic molecules; comparison of MO and VB theories. Hückel MO theory for conjugated  $\pi$ -systems. Polyatomic molecules, hybridisation and valence MOs of simple molecule like  $H_2O$ ,  $NH_3$ ,  $CH_4$ ,  $C_2H_6$  etc.

(12 Hours)

#### Unit – 2: *Ab-initio* Methods for Closed Shell Systems

Introductory treatment of semi-empirical and *ab-initio* calculations on molecular systems; the Hartree-Fock Self-Consistent Field Method; the generation of optimized orbitals, Koopman's theorem (The Physical Significance of Orbital Energies), electron correlation energy; density matrix analysis of the Hartree-Fock approximation, natural orbitals, matrix solution of the Hartree-Fock equations (Roothaan's equations); Hellman-Feynman theorem.

(12 Hours)

#### Unit – 3: Thermodynamics

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential, and entropies. Thermodynamics of open systems: partial molal properties, partial molal free energy, partial molal volume and partial molal heat content and their significances. Determination of these quantities. Concept of fugacity and determination of fugacity.

Non-ideal system: excess function for non ideal solutions. Activity, activity coefficient, Debye-Hückel theory for activity coefficient of electrolytic solution; determination of activity and activity coefficients; ionic strength.

(12 Hours)

#### Unit – 4: Non-equilibrium Thermodynamics

Thermodynamic criteria for non-equilibrium state, entropy production and entropy flow, energy balance equation for different irreversible processes (e.g. heat flow, chemical reaction etc.), transformation of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equation, microscopic, reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological system, coupled reactions.

(12 Hours)

#### Unit – 5: Solid State Chemistry

Perfect and imperfect crystals, intrinsic and extrinsic defect, point defect, line and plane defect, vacancies, Schottky and Frankel defects; thermodynamics of Schottky and Frankel defect formation, color center, non-stoichiometry defects. Metal insulators and semiconductors, electronic structure of solids-band theory, band structure of metals,

insulators and semi-conductors, doping semi-conductors,  $p$ - $n$  junction; superconductors; photoelectric effects; magnetic properties. Behaviour of substances in a magnetic field, effect of temperature: Curie and Curie-Weiss law, origin of magnetic moment, ferromagnetic, antiferromagnetic and ferromagnetic ordering, super exchange, magnetic domains, hysteresis.

(12 Hours)

**Reference Books:**

- Ira. N. Levine: Quantum Chemistry, Eds: 5<sup>th</sup>, PHI, 2000.
- A. K. Chandra: *Introductory Quantum Chemistry*, Eds: 4<sup>th</sup>, Tata McGraw Hill, New Delhi, 1994.
- P. Atkins and R. Friedman: *Molecular Quantum Mechanics*, Eds: 5<sup>th</sup>, Oxford University Press, 2011.
- T. Engle and P. Reid: *Quantum Chemistry and Spectroscopy*, Pearson, New Delhi, 2011.
- B. R. Puri, L. R. Sharma and M. S. Pathania, *Principle of Physical Chemistry*, Eds. 44<sup>th</sup>, Vishal Publishing Co., Jalandhar, 2010.
- P. Atkins and J. D. Paula, *Physical Chemistry*, Eds. 7<sup>th</sup>, Oxford University Press, New Delhi, 2002.
- R. S. Berry, S. A. Rice and J. Ross: *Physical Chemistry*, Eds: 2<sup>nd</sup>, Oxford University Press, New Delhi, 2007.
- S. R. Degroot, P. Mazur: *Non-Equilibrium Thermodynamics*, North Holland Publication, Amsterdam, 1961.
- C. N. R. Rao and J. Gopalakrishnan: *New Direction in Solid State Chemistry*, Cambridge University Press, 1997.
- A. R. West: *Solid State Chemistry and Its Applications*, John Wiley & Sons, 1989.
- L. Smart and E. Moore: *Solid State Chemistry*, Chapman and Hall, 1992.

# CHM T 512: Bio-Inorganic & Nuclear Chemistry

Credits: Theory-04

Theory: 60 Hours

## Unit – 1: Bio-inorganic Chemistry – I

Transport and storage of dioxygen: Active site structures and bio functions of O<sub>2</sub>-uptake proteins: hemoglobin, myoglobin, hemocyanin and hemerythrin; model synthetic dioxygen complexes. Chelato therapy. Electron transfer in biology: Active site structures and functions of cytochromes, cytochrome *c*; iron-sulfur proteins (rubredoxin, ferredoxines), organic-redox protein cofactors – FAD, NAD, FMN, ubiquinone; blue copper proteins, HIPIP. Respiratory electron transport chain, cytochrome *c* oxidase. Photosynthesis and chlorophylls, photosystem-I and photosystem-II and their roles in cleavage of water. Model systems. Biological and abiological nitrogen fixing systems, model study.

(12 Hours)

## Unit – 2: Advanced Bio-inorganic Chemistry – II

Metal ion interactions with purine and pyrimidine bases, nucleosides, nucleotides and nucleic acids, DNA and RNA, metal ions in genetic information transfer.

Redox enzymes: Catalase, peroxidase, super oxide dismutase (SOD), cytochrome P-450,

Nitrogen cycle enzymes: NO<sub>x</sub> reductases, nitric oxide synthases (NOS), ascorbate oxidase, aldehyde oxidase, sulfite oxidase, xanthine oxidase, nitrogenase, P and M clusters in nitrogenase, transition metal dinitrogen complexes and insights into N<sub>2</sub> binding, reduction to ammonia.

(12 Hours)

## Unit – 3: Enzymes

Zinc enzymes, magnesium enzymes, iron enzymes, carbonic anhydrase, xanthine oxidase, aldehyde oxidase, cobalt containing enzymes, Mo and tungsten enzymes, Vitamin B-12

**Zinc in Transcription:** Zinc fingers, zinc thiolate clusters.

**Calcium Signaling Protein:** Calmodulin protein and Ca<sup>2+</sup> ion pump

**Biological Cycle:** Nitrogen cycle, hydrogen cycle, in vivo and vitro nitrogen fixation

**Sensors:** Iron protein as sensor, Copper sensor, protein that sense copper and zinc level

**Other Application:** Biomineralization, cancer treatment, antiarthristis drugs

**Contribution of Individual Elements in Biological Function:** Na, K, Li, Mg, Ca, Se, Mn, Fe, Co, Ni, Cu, Zn, Mo, W, Si, Pt, Au

(12 Hours)

## Unit – 4: Inorganic Photochemistry

Introduction to inorganic photochemistry, photophysical and photochemical process. Excitation modes in transition metal complexes, fate of photo-excited species, fluorescence and phosphorescence applied to Inorganic systems, intramolecular energy transfer, vibrational relaxation, internal conversion and intrasystem crossing, quantum yield, decay

fluorescence. Fluorescence quenching, Stern-Volmer equation. Photochemical process: photo substitution and photoelectron transfer reactions in Co, Cr, Ru and Rh complexes.

(12 Hours)

### Unit – 5: Nuclear Chemistry & Radiochemical Analysis

**Nuclear models:** Nuclear stability, terrestrial abundance and distribution, relativistic effect, electronic configuration, oxidation states, aqueous-, redox- and complex- chemistry; Nuclear forces, liquid drop model, shell model, Fermi gas model; magic numbers, nuclear spin and nuclear isomerism. **Nuclear reactions:** Energetics, mechanism and models of nuclear reactions. Nuclear fission and nuclear fusion, fission products and fission yields. Interactions of radiation with matters, chemical effects of nuclear transmutation (elementary idea), Nuclear reactors and particle accelerators.

**Radioactive Techniques:** Detection and measurement of radiation- GM ionization and proportional counters. Study of chemical reactions by tracer techniques, isotope exchange and kinetic isotope effect. Radiometric analysis: Isotope dilution analysis, age determination, neutron activation analysis (NAA) and their applications. Radiation hazards and safety measures.

(12 Hours)

### References Books:

- S. J. Lippard and J. M. Berg: *Principles of Bioinorganic Chemistry*, University Science Books, Mill Valley, 1994.
- W. Kaim and B. Schwederski: *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*, John Wiley & Sons Inc., 1994.
- D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
- B. R. Puri, L. R. Sharma, and K. C. Kalia: *Principle of Inorganic Chemistry*, Milestone Publisher, New Delhi **2010**.
- D. L. Nelson, & M. M. Cox: *Lehninger's Principles of Biochemistry 7 Ed.*, W. H. Freeman
- H. J. Arnikar, *Essential of Nuclear Chemistry*, Wiley-Blackwell; 2nd Edition edition.
- *Hand Book of Nuclear Reactions*, edited by Vértes, A., Nagy, S., Klencsár, Z., Lovas, R.G., Rösch, F. , Springer
- J. E. Huheey, E. A. Keiter, R. L. Keiter, and O. K. Medhi: *Inorganic Chemistry Principle of Structure and Reactivity*, Eds: 4<sup>th</sup> Pearson, New Delhi, 2006.
- A. Das and G. N. Mukherjee, *Elements of Boi-inorganic Chemistry*.
- Ashim Kr. Das, *Boi-inorganic Chemistry*.

# CHM T 513: Pericyclic Reaction, Photochemistry and Free Radical Chemistry

Credits: Theory-04  
Theory: 60 Hours

## Unit – 1: Introduction of Pericyclic Reaction

Definition, Symmetry of  $\pi$  molecular orbital, Filling of electrons in  $\pi$  molecular orbital in conjugated polyenes, conjugated ions, Frontier Molecular Orbital Theory, Classification of Pericyclic reactions

(10 Hours)

## Unit – 2: Electrocyclic and Cycloaddition Reactions

**Electrocyclic Reactions:** Conrotatory and disrotatory motion in ring opening and ring closing reactions, Frontier Molecular Orbital (FMO) approach for Electrocyclic reactions, Correlation diagram of the Electrocyclic reactions with  $4n\pi$  and  $(4n + 2)\pi$  electronic systems, Woodward – Hoffmann rule for Electrocyclic system.

**Cycloaddition Reactions:** Theory of Cycloaddition reaction, Stereochemistry of Cycloaddition reaction, Diels-Alder reaction, 1, 3-Dipolar Cycloaddition reactions, Chelotropic reactions. Woodward – Hoffmann selection rule for Electrocyclic system.

(12 Hours)

## Unit – 3: Sigmatropic Rearrangement and Group Transfer Reactions

Definition, Classification of Sigmatropic Rearrangement, Mechanism of Sigmatropic Rearrangement, Various types of  $[m, n]$  Sigmatropic rearrangements, Cope, Oxy-Cope and Claisen Rearrangement. Ene Reactions and Group Transfer Reactions given by Diimide.

(12 Hours)

## Unit – 4: Photochemistry

**Basic Principle of Photochemistry and Reaction with Carbonyl compounds:** Introduction of Photochemistry-Jablonski Diagram, Quantum Yield calculation of photo chemical reaction, photosensitizer and quencher;  $\alpha$ -cleavage (Norrish type I & II) and  $\beta$ -cleavage reactions with carbonyl compounds, Intra- and Intermolecular Hydrogen abstraction reactions with carbonyl compounds, Photocycloaddition reactions (Paterno-Büchi Reaction).

**Photo Rearrangement, Photo Reduction, and Photo Isomerization Reactions:** Di-  $\pi$ -Methane Rearrangement, Aza-di-  $\pi$ -Methane Rearrangement, Photo reduction of carbonyl compounds, Cis-Trans Isomerization reactions with alkenes, Photochemistry of Dienes.

(14 Hours)

## Unit – 5: Free Radical Reactions

Principles, Generation of free radicals, Formation of Carbon-Halogen bonds (Hunsdiecker reaction), Formation of Carbon-Carbon bonds (addition to carbon-carbon double bonds, Acyloin condensation reaction, Eglinton reaction). Formation of Carbon-Nitrogen bonds (Barton Reaction and Hoffmann-Loeffler-Freytag Reaction).

(12 Hours)

### Reference Books:

- J. Singh & J. Singh: *Photochemistry and Pericyclic Reactions*, New Age International (P) Ltd., 2007
- B. B. Woodward and Hoffman: *Conservation of Orbital Symmetry*, Verlag Chemie Academic Press, 1971.
- W. Carruthers: *Some Modern Methods of Organic Synthesis*, Cambridge University, Press, 1993.

## CHM P 511: Physical Chemistry Practical – II

Credits: 02  
Lab: 60 Hours

- (i) Conductometry
- (a) The measurement of electrical conductance for the determination of the equivalent conductance at infinite dilution.
  - (b) Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulfate using Debye-Hückel's limiting law.
  - (c) To verify Debye-Hückel limiting law for strong electrolyte.
- (ii) (a) Rate of the hydrolysis of sucrose using polarimeter.  
(b) Polarizability from refractive index measurement.
- (iii) Potentiometry/pHmetry
- (a) Determination of pK<sub>a</sub> of poly-basic acid with the pH meter.
  - (b) To determine the pH of various mixtures of acetic acid and sodium acetate in aqueous solutions and hence determine the dissociation constant of the acid.
- (iv) Determination of the transport number by moving boundary method.
- (v) IR and Raman spectroscopy of the solvent mixture.

### Reference Books:

- A. M. James and F. E. Prichard: *Practical Physical Chemistry*, Longman.
- B. P. Levi: *Findley's Practical Physical Chemistry*,
- R. C. Das and B. Behera: *Experimental Physical Chemistry*, Tata McGraw Hill.
- D. P. Shoemaker, G. W. Garland and J. W. Niber: *Experimental Physical chemistry*, Mc Graw Hill Interscience.
- A. J. Elias: *A collection of Interesting General Chemistry Experiments*, University Press, India.
- J. Rose: *Advanced Physico-Chemical Experiments*, Sir Isaac Pitman & Sons Ltd, London.
- J. B. Yadav: *Advanced Practical Physical Chemistry*, Krishna Prakashan Media (P) Ltd. Meerut.

## CHM P 512: Inorganic Chemistry Practical – II

Credits: 02  
Lab: 60 Hours

### A. Analytical Chemistry:

- Analysis of Ores: Felspar , bauxite, Rocks available in that region.
- Analysis of Soil sample, animal feeds, soil micronutrients, milk powder for Ca, Fe and P content.
- Separation of Mixture: Chromium (III) and Mn(II) in a mixture, Iron (III) and Cu(II) in a mixture, Iron(III) and Al(III) in a mixture

At least one ore/ mineral/concentrate and one alloy should be analyzed during the laboratory session.

### B. Preparations of Complex (At Least eight samples)

Preparation of selected inorganic compound and their studies by I.R. electronic spectra, Mössbauer and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds

1. bis(ethylene)nickel(II)thiosulphate,
2. tris(acetylacetonato)manganese(III), tris(acetylacetonato)Aluminium(III), tris(acetylacetonato)iron(II), tris(acetylacetonato)copper(II),
3. Hexaminecobalt(III)chloride,
4. Mercury tetrathiocyanatocobaltate(II),
5. Copper(II) biguanide
6. Mn<sub>12</sub> Acetate Single Molecule Magnet
7. Preparation of copper glycine complex- cis and trans bis- (glycinato) copper (II).
8. Preparation of N, N-bis-(salicyldehyde) ethylenediamine, Co(salen), Mn(salen), determination of O<sub>2</sub> absorption by Co(salen), reaction of oxygen adduct with CHCl<sub>3</sub> (deoxygenation).
9. VO(acac)<sub>2</sub>
10. cis-K [Cr(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub> (H<sub>2</sub>O)<sub>2</sub>]
11. Na[Cr(NH<sub>3</sub>)<sub>2</sub> (SCN)<sub>4</sub>]
12. K<sub>2</sub>[Fe(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>]

### Reference Books:

- *Vogel's Textbook of Quantitative Analysis*, Revi Mendham, ELBS.
- W.L. Jolly, *Synthesis and Characterization of Inorganic Compounds*, Prentice Hall.

## SEMESTER – IV

### CHM T 521: Molecular Spectroscopy

Credits: Theory-04  
Theory: 60 Hours

#### Unit – 1: Unifying Principles

Electromagnetic radiation, interaction of electromagnetic radiation with matter, absorption, emission, transmission, reflection, refraction, dispersion, polarization, and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, result of the time dependent perturbation theory, transition moment selection rules, intensity of spectral line. Born-Oppenheimer approximation, rotational, vibrational, and electronic energy levels. Fourier Transform Spectroscopy.

(10 Hours)

#### Unit – 2: Microwave Spectroscopy

**Rotational spectroscopy:** Classification of molecules, rigid rotor model, selection rule, intensity of spectral line, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect nuclear and electron spin interaction and effect of external field. Applications (determination of bond lengths of diatomic and linear triatomic molecules *etc.*)

(10 Hours)

#### Unit – 3: Vibrational Spectroscopy

**A. Infrared Spectroscopy:** Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P, Q, R branches. Breakdown of Oppenheimer approximation; vibration of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factor affecting the band positions and intensities, far IR region, metal-ligand vibrations, normal co-ordinate analysis. Fourier Transform Infra-red Spectroscopy (FTIR)

**B. Raman Spectroscopy:** Classical and quantum theories of Raman Effect, pure rotational, vibrational, and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti-stokes Raman spectroscopy (CARS).

(10 Hours)

#### Unit – 4: Electronic Spectroscopy

**A. Atomic Spectroscopy:** Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

**B. Molecular Spectroscopy:** Energy levels, molecular orbitals, vibronic transition, vibrational progressions and geometry of excited state, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, spectra of transition metal complex, charge transfer spectra.

**C. Photoelectron Spectroscopy:** Basic principle; photo-electronic effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA, basic idea Auger electron spectroscopy.

(10 Hours)

### Unit – 5: Magnetic Resonance, Photoacoustic, and Mössbauer Spectroscopy

**A. Nuclear Magnetic Resonance Spectroscopy:** Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurement, factor influencing chemical shift, deshielding, spin-spin interaction, factor influencing coupling constant 'J'. Classification (ABX, AMX, ABC, A2B2 etc), spin decoupling; basic idea about instrument, NMR studies of nuclei other than proton –  $^{13}\text{C}$ ,  $^{19}\text{F}$ , and  $^{31}\text{P}$ ; FT NMR, advantage of FT NMR, use of NMR in medical diagnostics.

**B. Electron Spin Resonance Spectroscopy:** Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

**C. Nuclear Quadrupole Resonance Spectroscopy:** Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting, applications.

**D. Photoacoustic Spectroscopy:** Basic principles of photoacoustic spectroscopy (PAS). PAS-gases and condensed system, chemical and surface applications.

**E. Mössbauer Spectroscopy:** Basic principles, spectral parameters and spectrum display. Application of technique to the studies of (i) bonding and structure of  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  compounds – nature of M-L bond, coordination number, structure and (ii) detection of oxidation state and inequivalent MB atom.

(20 Hours)

#### Reference Books:

- T. Engle and P. Reid: *Quantum Chemistry and Spectroscopy*, Pearson, New Delhi, 2011.
- B. K. Sharma: *Instrumental Methods of Chemical Analysis* - 9th Edition.
- William Kemp: *Organic Spectroscopy* –3rd Edition.
- C. N. Banwell and E. M. McCash: *Fundamentals of Molecular Spectroscopy*, Ed. 4<sup>th</sup>, Tata McGraw-Hill, 1994.
- G. M. Barrow: *Introduction to Molecular Spectroscopy*

## **CHM P 522: Project and Dissertation**

**Credits: 08**

Each student is assigned to a faculty supervisor to carry out a research project. They will be trained in searching research literature as well as experimental and computational work specific to the chosen research problem. On the basis of partial fulfilment of project report the student may go other University/Institute for project work. At the end of the project they will submit a report of the work done and make a presentation for evaluations.

## LIST OF ELECTIVE PAPER

| S. No. | Course Code | Course Structure | Title of Paper                                   | Credit |
|--------|-------------|------------------|--|--------|
| 1      | CHM T 601   | Elective         | Mathematics for Chemist                          | 3      |
| 2      | CHM T 602   | Elective         | Biology for Chemist                              | 3      |
| 3      | CHM T 603   | Elective         | Industrial Chemistry                             | 3      |
| 4      | CHM T 604   | Elective         | Instrumental Methods of Analysis                 | 3      |
| 5      | CHM T 605   | Elective         | Basic of Materials Chemistry                     | 3      |
| 6      | CHM T 606   | Elective         | Introduction to Nanomaterials and Nanotechnology | 3      |
| 7      | CHM T 607   | Elective         | Polymers Chemistry                               | 3      |
| 8      | CHM T 608   | Elective         | Bioorganic and Drug Chemistry                    | 3      |
| 9      | CHM T 609   | Elective         | Advanced Heterocyclic Chemistry                  | 3      |
| 10     | CHM T 610   | Elective         | Chemistry of Natural Products                    | 3      |
| 12     | CHM T 611   | Elective         | Solid State Chemistry                            | 3      |
| 13     | CHM T 612   | Elective         | Advanced Synthetic Organic Chemistry             | 3      |

**Note:** M.Sc. in Chemistry students have to opt total three elective papers (commonly name as Discipline Specific Elective) from the above list of elective courses from the second semester onwards. Students have to choose only that elective courses, those are offered by the Departmental faculty members in the respective semesters in the running academic years.

## CHM T 601: Mathematics for Chemist

Credits: Theory-03  
(45 Hours)

### A. Mathematics for Chemist

#### Unit – 1: Vectors and Matrix Algebra

**Numbers:** Real and Complex number

**Vectors:** Vectors, dot, cross and triple product etc. The gradient, divergence and curl. Vector calculus, Gauss' theorem, divergence theorem *etc.*

(9 Hours)

#### Unit – 2: Matrix Algebra

Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (symmetric, screw-symmetric, Hermitian, screw-Hermitian, unit, diagonal, unitary *etc.*) and their properties. Matrix equations; homogeneous, non-homogeneous linear equation and conditions for the solution, linear dependence and independence. Introduction of vector spaces, matrix eigenvalues and eigenvectors, diagonalization, determinants (examples from Hückel theory). Introduction to tensors; polarizability and magnetic susceptibility as examples.

(9 Hours)

#### Unit – 3: Differential and Calculus

**Differential:** Functions, continuity and differentiability, rules for differentiation, application of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution *etc.*), exact and inexact differentials with their application to the thermodynamic properties.

**Partial Differential:** Function of several variables, partial differentiation, co-ordinate transformation (e.g. Cartesian to spherical polar).

**Integral calculus:** basic rules for integration, integration by parts, partial fraction and substitution, reduction formulae, applications of integral calculus.

(9 Hours)

#### Unit – 4: Elementary Differential Equations

Ordinary first- and second-order differential equations. Partial differential equations. Solution of inexact differential equations by the method of integrating factors. Power series and extended power series solutions. Numerical solutions. Special functions: Hermite, Legendre and Laguerre polynomials, recursion relations.

(9 Hours)

#### Unit – 5: Probability and Curve Sketching

Permutation & Combination. Probability. Stirling's approximation. Lagrange multipliers. Curve sketching and curve fitting; Introduction to Fourier series and Fourier transforms.

(9 Hours)

#### Reference Books:

- R. G. Mortimer: *Mathematics for Physical Chemistry*, Academic Press.
- F. Diniels: *Mathematical Preparation for Physical chemistry*, McGraw Hill.

## CHM T 602: Biology for Chemist

Credits: Theory-03  
Theory: 45 Hours

### Unit – 1: Cell Structure & Functions

Structure of prokaryotic and eukaryotic cells, intracellular organelles and their function, comparison of plant and animal cells. Overview of metabolic processes-catabolism and anabolism; ATP the biological energy currency. Origin of life – unique property of carbon, chemical evolution and rise of living systems. Introduction to biomolecules, building blocks of bio-molecules.

(9 Hours)

### Unit – 2: Carbohydrates

Conformation of monosaccharides, structure and function of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars, N-acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides – cellulose, and chitin; storage polysaccharides – starch and glycogen. Structure and biological functions of glucosaminoglycans or mucopolysaccharides. Carbohydrates of glycoproteins glycolipids. Role of sugar in biological recognition. Blood group substances. Ascorbic acid, carbohydrate metabolism – Krebs' cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis pentose phosphate pathway.

(9 Hours)

### Unit – 3: Lipids

Fatty acids, essential fatty acids, structure and function of triglycerols; glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins – composition and function, role in atherosclerosis. Properties of lipids, aggregates – micelles, bilayers, liposomes and their possible biological function. Biological membranes, fluid mosaic model of membranes structure. Lipid metabolism  $\beta$ -oxidation of fatty acids.

(9 Hours)

### Unit – 4: Amino Acids

**Amino Acids, Peptides and Proteins:** Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing, secondary structure of proteins, force responsible for holding of secondary structure.  $\alpha$ -helix,  $\beta$ -sheet, super secondary structure, triple helix structure of collagen. Tertiary structure of proteins, folding and domain structure. Quaternary structure. Amino acid metabolism, degradation and biosynthesis of amino acids, sequence determination, chemical/enzymatic/mass spectral racemization detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).

(9 Hours)

### Unit – 5: Nucleic Acids

Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis of heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono- and tri- nucleosides.

(12 Hours)

### Reference Books:

- A. L. Lehninger: *Principle of Biochemistry*, Worth Pub. Shers.
- L. Stryer and W. H. Freeman, *Biochemistry*
- J. David Rawn: *Biochemistry*, Neil Patterson.

## CHM T 603: Industrial Chemistry

Credits: Theory-03  
Theory: 45 Hours

### Unit – 1: Water and Its Treatment

Sources of water, chlorinated and nonchlorinated water, chemical method of sterilization: precipitation method, Aeration, ozonisation, chlorination, chloramines process, potassium permanganate method, Physical method of sterilization: Boiling, exposure to sunlight, hard and soft water, Types of hardness, temporary and permanent hardness, water softening, cold and hot lime soda process, zeolite process, ion exchange process, removal of iron, silica, and dissolved oxygen from water for industrial purposes, water for boiler uses, water analysis.

(9 Hours)

### Unit – 2: Glass and Rubbers

**Glass:** physical and chemical properties of glass, constituents in glasses, raw materials, manufacturing of glasses, optical glass, borosilicate glass, lead glass, colored glass, opal glass, safety glass, fiber glass.

**Natural and Synthetic Rubber:** classification of rubber, natural and synthetic rubber.

(9 Hours)

### Unit – 3: Chemical Fertilizers

Classification of fertilization, nitrogenous fertilizers, method of production and its action- ammonium nitrate, ammonium sulphate, urea, calcium cyanamide, ammonium chloride, phosphate rock, normal super phosphate, triple super phosphate.

(9 Hours)

### Unit – 4: Petroleum

Classification of petroleum, composition of petroleum, mining of petroleum, refining of petroleum, octane rating, octane number and antiknock compound, cetane number, production of gases, crude naphtha, benzene, kerosene oil, fuel oil, lubricating oil, paraffin wax and black tarry after refining. Cracking: thermal cracking, hydrocracking, and fluid catalytic cracking.

(9 Hours)

### Unit – 5: Fibers and Dyes

**Synthetic Fibers:** Preparation of fibers- Nylons, Nylon-66, Nylon-6, Nylon-11, Nylon-610, Nylon-8, polyethylene terephthalate, orlon, saran, vinyon, taflon.

**Synthetic Dyes and Dyeing:** Requisites of true dyes, sensation of color, witt's theory, chromophores, auxochromes: batho-, hypso-, hyper-, and hypochromic shifts; classification of dyes: acid dyes, basic dyes, adjective dyes, vat dyes, ingrain dyes, sulfur dyes, pigment dyes, nitroso dyes, nitro dyes, azo dyes, xanthenes dyes, applications of dye.

(9 Hours)

### Reference Books:

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
- R.M. Felder, R.W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
- J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
- S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.

## **CHM T 604: Instrumental Methods of Analysis**

**Credits: Theory-03**

**Theory: 45 Hours**

### **Unit – 1: Molecular Spectroscopy**

Nature of electromagnetic radiation, electromagnetic spectrum, atomic, molecular and vibrational energy levels, basic instrumentation- source of radiation, monochromator, sample cells, absorber, detector, UV-Vis detector, photomultiplier, IR detector, display and recorder, single and double beam spectrophotometer, Beer Lambert law, deviation from beers law, ultraviolet and visible spectroscopy, Fluorescence and phosphorescence spectrophotometer, Fourier transform infrared spectrometer and Raman spectrometer, instrumentation, techniques and application.

**(9 Hours)**

### **Unit – 2: Atomic Spectroscopy**

Flame emission spectrometry, atomic absorption spectroscopy- principle, instrumentation, Source in AAS – Hollow cathode lamp, electrode less discharge lamp, burners, nature and property of flame, interference in AAS, difference between AAS and FES, ICP.

**(9 Hours)**

### **Unit – 3: Thermal Analysis**

Types of thermal method, Thermogram, thermogravimetric analysis(TGA), differential thermal analysis(DTA), differential scanning calorimetry (DSC), schematic diagram for TGA and DTA instruments and their working principle, factors affecting thermogram like geometry of sample holder, furnace atmosphere, heating rate, particle size, packing of sample, weight of sample, analysis of metals or oxide in mixture, application of TGA and DTA.

**(9 Hours)**

### **Unit – 4: Chromatography**

Principles of chromatographic separation, classification of Chromatographic Techniques: adsorption, partition, ion exchange and size exclusion chromatography, theory of chromatographic separation, distribution coefficient, retention time, sorption, theory of column efficiency and resolution, separation factor, retention factor. – working principle and application of Column chromatography, ion exchange chromatography, paper chromatography, Thin layer chromatography (TLC) & HPTLC: techniques and application. - Gas Chromatography and high performance liquid chromatography: Van Deemter equation, retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation efficiency and resolution, instrumentation and application.

**(9 Hours)**

### **Unit – 5: Electroanalytical Techniques**

Electrochemical cells, current potential relationship, mass transfer by migration, convection and diffusion, Electrogravimetry, voltam-metry, polarography, reference electrode, working electrode, auxiliary electrode, dropping mercury electrode, current potential curve, limiting current, coulometry, conductometry methods, instrumentation, techniques and application. Amperometric titration, effect of electroactive and reagent on amperometric curve and its advantage, rotating platinum electrode, biamperometric titration and its advantage, fluorimetry and phosphorimetry.

**Reference Books:**

- Arthur I. Vogel: *A Test book of Quantitative Inorganic Analysis* (Rev. by G.H. Jeffery and others) 5<sup>th</sup> Ed. The English Language Book Society of Longman .
- Hobert H. Willard et al: *Instrumental Methods of Analysis*, 7<sup>th</sup> Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Gary D. Christian: *Analytical Chemistry*, 6<sup>th</sup> Ed. John Wiley & Sons, New York, 2004.
- C. Daniel Harris: *Exploring Chemical Analysis*, Ed. New York, W.H. Freeman, 2001.
- S. M. Khopkar: *Basic Concepts of Analytical Chemistry*, New Age, International Publisher, 2009.
- D. A. Skoog, F. J. Holler and T. A Nieman: *Principles of Instrumental Analysis*, Thomson Asia Pvt. Ltd. Singapore.
- O. Mikes & R. A. Chalmes: *Laboratory Hand Book of Chromatographic & Allied Methods*, Elles Harwood Ltd. London.
- R. V. Ditts: *Analytical Chemistry – Methods of separation*.

## CHM T 605: Basic of Materials Chemistry

**Credits: Theory-03**  
**Theory: 45 Hours**

### Unit – 1: Chemical Crystallography

**Introduction:** Space lattice, crystal point groups, space group (working knowledge), stereographic projections, packing in solids, crystal structures of representative systems, silicates and zeolites, cements, glasses, quasicrystals, nanostructures.

**Bonding in Solids and Crystal Energetics:** Crystal classifications, Madelung constant and Lattice energy.

**(9 Hours)**

### Unit – 2: Characterization Techniques for Solids

X-ray diffraction, electron microscopy (SEM, TEM, AFM), thermal techniques (TG, DTA, DSC), spectroscopic techniques (Mössbauer, IR, UV-VIS), and physical property measurement techniques (magnetic moments-VSM/SQUID, electrical resistivity – two / four probe methods and thermal conductivity, optical band gap, XPES, XAS.

**(9 Hours)**

### Unit – 3: Electronic and Magnetic Properties Solids

**Electronic Properties and Band Theory of Solids:** Free electron theory of metals, Band theory of solids, Bloch theorem, Kroning-Penne model, refinement of simple band theory-  $k$ -space and Brillouin Zones, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doped semiconductors,  $p$ - $n$  junctions.

**Magnetic Properties Solids:** Behaviour of substances in a magnetic field, effect of temperature: Curie and Curie-Weiss law, origin of magnetic moment, ferromagnetic, antiferromagnetic and ferromagnetic ordering, super exchange, magnetic domains, hysteresis. Introduction of superconductors, Meissner effects, basic concepts of BCH theory.

### Unit – 4: Defects and Phase Transitions

**Defects, Nonstoichiometry and Diffusion:** Point defects, dislocations, extended defects, clusters and aggregates, color centers, nonstoichiometry of compounds, diffusion mechanisms, Fick's law, Kirkenall effect.

**Phase Transitions:** Critical phenomena, variety of phase transitions (ordered-disorder, Martensite-austenite, spinoidal decompositions *etc*), liquid crystals, structure-property relations (magnetic, electrical, superconductivity, optical and thermal).

### Unit – 5: Preparative Techniques

**Reactivity of Solids:** Decomposition and reactivity, solid state reactions, sintering process, reaction kinetics, organic solid reactions.

**Conventional Techniques:** Powder mixing, fusion, precipitation from solution, modern need for improved synthetic routes, crystal growth and thin film techniques.

**Chemical Routes:** Wet-chemical (Oxidation-reduction for metal nanoparticles) methods, self assembly methods, reverse micelles route, biomimetic, sonochemical, and electrochemical approaches.

**Sol-Gel Synthesis:** Colloids, cation hydrolysis and sol formation, gel precipitation, sol-gel process for colloids, synthesis and physical properties of metal alkoxides, development of sol-gel process from alkoxides, derived coatings, fibers and monodispersed submicron/nanostructured oxide powders, ormosils, sialons.

**Hydrothermal/Solvothermal Approach:** Forced hydrolysis at elevated temperatures and pressures, hydrothermal reactions using salt solutions, metal reactants and reactions involving phase transformation.

**Precursor Technique:** Citrate-gel process, metallo-organic precursors, metal alkoxides.

**Gas Phase Reactions:** Gas-phase nucleation, flame hydrolyzed powders, direct - nitridation and carbothermic reduction, non-plasma gas phase reactions, plasma reactions, electron beam evaporation.

**(12 Hours)**

#### **Reference Books:**

- A. R. West: *Solid State Chemistry and Its Applications*, John Wiley & Sons, 1989.
- L. Smart and E. Moore, *Solid State Chemistry*, Chapman and Hall, 1992.
- A. K. Cheetham and P. Day: *Solid State Chemistry Compounds*, Clarendon Press, Oxford 1992.
- C. N. R. Rao and J. Gopalkrishnan: *New Directions in Solid State Chemistry*, Cambridge Univ. Press 1997.
- R. E. Newnham, *Structure Property Relations*, Springer-Verlag, 1987

# CHM T 606: Introduction to Nanomaterials and Nanotechnology

Credits: Theory-03  
Theory: 45 Hours

## Unit – 1: Nanoscience and Nanotechnology

**Introduction:** Underlying physical principles of nanotechnology: *Nanostructured Materials: Size is Everything*. Fundamental physicochemical principles, size and dimensionality effects; quantum confinement; properties dependent on density of states; single electron charging, central importance of nanoscale morphology. Societal aspects of nanotechnology: health, environment, hype and reality.

**Type of Nanostructures:** Definition of a nano system; one dimensional (1D), two dimensional (2D), three dimensional (3D) nanostructured materials; quantum dots; quantum wire, and core/shell structures.

(9 Hours)

## Unit -2: The Basic Tools of Nanotechnology

Electron microscopy (SEM, TEM with EDX analysis) and X-ray diffraction, A brief historical overview of atomic force microscopy (AFM); an introduction and basic principles & applications of XPS, FTIR spectrophotometers; UV-VIS principle and application for band gap measurement.

(9 Hours)

## Unit – 3: Synthesis of Nanomaterials

Top down and bottom up approaches to synthesis of nanomaterials:

**Chemical Routes for Synthesis of Nanomaterials:** Chemical precipitation and co-precipitation; sol-gel synthesis; microemulsions or reverse micelles; solvothermal synthesis; thermolysis routes, microwave heating synthesis biomimetic and electrochemical approaches; sonochemical synthesis; photochemical synthesis; synthesis in supercritical fluids.

**Physical Routes for Preparation of Nanomaterial:** Inert gas condensation, arc discharge, RF plasma, plasma arc technique, ion sputtering, laser ablation, laser pyrolysis, spray pyrolysis, ball milling, molecular beam epitaxy, chemical vapour deposition method, Langmuir-Blodgett (LB) films, spin coating and electro deposition.

(9 Hours)

## Unit – 4: Nanomaterials and Properties

Synthesis and size dependent properties (mechanical, physical and chemical properties) of carbon nanotubes (CNT); metals (Au, Ag); metal oxides (TiO<sub>2</sub>, CeO<sub>2</sub>, ZnO); semiconductors (Si, Ge, CdS, ZnSe); dilute magnetic semiconductor.

(9 Hours)

## Unit -5: Applications of Nanomaterials

Basic ideas of nanodevices (molecular electronics and nanoelectronics, and quantum electronic devices); CNT based transistor and field emission display; biological applications; biochemical sensor; membrane based water purification, energy storage devices, catalysis and various related fields.

**(12 Hours)**

**Reference Books:**

- T. Pradeep, *Nano: The Essentials*, Tata McGraw-Hill, New Delhi, 2007.
- G. Cao, *Nanostructures and Nanomaterials – Synthesis, Properties and Applications*, Imperial College Press, London, 2004,
- C. N. R. Rao, A. Muller and A. K. Cheetham, *The Chemistry of Nanomaterials*
- G. L. Hornyak, J. J. Moore, H. F. Tibbals, and J. Dutta: *Fundamentals of Nanotechnology*, CRC Press, 2009

## CHM T 607: Polymers Chemistry

Credits: Theory-03  
Theory: 45 Hours

### Unit – 1: Introduction

Importance of polymers. Basic Concept: monomers, repeat units, degree of polymerization; linear, branched, and network polymers (block-copolymer, dendrimer etc.); classification of polymers. Polymerization: condensation, addition, radical, chain- ionic- and co-ordination-, and co-polymerization; polymerization condition and polymer reaction; polymerization in homogeneous and heterogeneous systems.

(9 Hours)

### Unit– 2: Polymer Characterization Techniques

Polydispersion-average molecular weight concept; number, weight and viscosity average molecular weights. Polydiversity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End group, viscosity, light scattering, osmotic, and ultracentrifugation methods. Analysis and testing of polymers-chemical analysis of polymers. Spectroscopic methods, X-ray diffraction, microscopy studies. Thermal analysis and physical testing tensile strength, fatigue, impact, tear resistance, hardness and abrasion resistance analysis.

(9 Hours)

### Unit – 3: Structure and Properties

Morphology and order in crystalline polymers – configuration of polymer chains; crystal structure of polymers; morphology of crystalline polymers; strain-induced morphology; crystallization and melting polymer structure and physical properties – crystalline melting point,  $T_m$ , melting points of homogeneous series effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature,  $T_g$ , relationship between  $T_m$  and  $T_g$ , effect of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Properties requirements for polymer utilization.

(9 Hours)

### Unit – 4: Polymer Processing

Plastic, elastomers and fibres, compounding; processing techniques- calendaring, die casting, rotational casting, film casting, injection casting, blow moulding, extraction moulding, thermoforming, foaming, reinforcing, and fibre spinning.

(9 Hours)

### Unit – 5: Properties of Commercial Polymers

Polyethylene, polyvinyl chloride, polyamide, polyester, phenolic resins, epoxy resins and silicone polymers. Functional polymers – fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin, and blood cells.

(9 Hours)

### Reference Books:

- Fred W. Billmeyer: *Textbook of Polymer Science*, Eds: 3<sup>rd</sup>, Wiley-India, New Delhi, 2012.
- A Ravve: *Principle of Polymer Chemistry*, Eds. 3<sup>rd</sup>, Springer Science + Business Media, New York, 2012.
- J. M. G. Cowie: *Physics and Chemistry of Polymers*, Blackie Academic and Professional.
- H. R. Alcock and F. W. Jamieson: *Contemporary Polymer Chemistry*, Prentice Hall.
- V. R. Govarikar, N. V. Viswanathan, and J. Sreedhar: *Polymer Science*, Wiley-Eastern.

# CHM T 608: Bioorganic and Drug Chemistry

**Credits: Theory-03**

**Theory: 45 Hours**

## **Unit – 1: Overview of Bioorganic Chemistry**

**Introduction:** Definition of bioorganic chemistry, Border line of bioorganic chemistry and inter disciplinary area between chemical and biology, Weak interaction in organic and biological world, Molecular Recognition.

**Chemistry of the Living Cell:** The structure of prokaryotic and Eukaryotic cells, Composition of living cells:

**(9 Hours)**

## **Unit – 2: Carbohydrates, Proteins, Lipids, and Nucleic Acids**

**Carbohydrates:** Introduction, Reactions of Monosaccharides, Interconversions, Ring structure of aldoses and ketoses, Confirmation of Monosaccharides, Disaccharides: Structure, synthesis and properties.

**Proteins:** General structure & classification of amino acids, Abbreviation of amino acids, Essential and non essential amino acids, Synthesis of amino acids, Isoelectric point, Acid and base properties of amino acids. Protein: Naturally occurring peptides, Modern methods of peptide synthesis with protection and deprotection, Determination of sequences and basic units of a poly peptides or proteins, C- & N-terminus detection by chemical methods, Primary, secondary, tertiary and quaternary structures of proteins, Enzyme active sites, allosteric sites, and mechanism of their actions e.g. chymotrypsin, carboxypeptidase, lipases etc.

**Lipids:** Lipid structure- acylglycerols, phosphoglycerides and sphingolipids, Biological importance of fatty acids and lipids, Bio- and chemical Synthesis of lipids.

**Nucleic Acids:** Definition, structure and properties, base pairing, double helices, Genetic information storage, transmission and gene expression, Nucleotides and Nucleosides: Similarities and differentiation, Structure of DNA & RNA. Types of mRNA, tRNA and rRNA, Replication, transcription and translation, Genetic code, Protein biosynthesis.

**(12 Hours)**

## **Unit – 3: Analogy Between Biochemical and Organic reactions**

Introduction to metabolism (catabolism, anabolism). ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change. Agents for transfer of electrons in biological redox systems:  $\text{NAD}^+$ , FAD. Conversion of food to energy: Outline of catabolic pathways of carbohydrate- glycolysis, fermentation, Krebs cycle. Overview of catabolic pathways of fat and protein. Interrelationship in the metabolic pathways of protein, fat and carbohydrate. Caloric value of food, standard caloric content of food types.

**(9 Hours)**

## **Unit – 4: Overview of Drug Chemistry and Basics of Drug Action**

Definition, classification and nomenclature of drugs, Preliminary idea of drug action: Interaction (Weak interaction in drug molecules, Chirality and drug action), Receptorology

(Drug-receptor interactions, Enzyme kinetics in drug action, Enzyme inhibitors (Drug action through enzyme inhibition), Nucleic acids as targets for drug actions, NA-Alkylation, NA-strand breaking and their importance in drug action, Drug metabolism, drug deactivation and elimination.

(8 Hours)

#### Unit – 5: Pharmaceutical Compounds: Structure and Importance

Classification, structure and therapeutic uses of antipyretics: Paracetamol (with synthesis), Analgesics: Ibuprofen (with synthesis), Antimalarials: Chloroquine (with synthesis). An elementary treatment of Antibiotics and detailed study of chloramphenicol, Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine).

(7 Hours)

#### Reference Books:

- L. Stryer: *Biochemistry*, 4<sup>th</sup> Edition W. H. Freeman and Co. 1995.
- S. Zubay: *Biochemistry*, Addison-Wesely 1983.
- J. Mann; R.S. Davidson: *Natural Products: Chemistry and Biological Significance*
- H. Dugas: *Bioorganic Chemistry Frontiers Vol. 2*, ed. Springer-Verlag, 1990.
- E. E. Tamlen: *Bioorganic Chemistry*, Academic Press, 1977.
- M. Bodansky: *Peptide Chemistry: A Practical Textbook*, Springer-Verlag 1988.
- *Bioorganic Chemistry: A chemical approach to enzyme action*, Springer-Verlag 1989.
- W. Saenger: *Principles of Nucleic acid structures*, Springer-Verlag 1984.
- G. R. Chatwal: *Medicinal Chemistry*
- A. Kar: *Medicinal Chemistry*, Wiley, 2000.
- D. Lednicer: *Strategies for Organic Drug Synthesis and Design*, John Wiley 1998.
- G. R. Chatwal: *Synthetic Drugs*, Himalaya, New Delhi 1995.
- S. Hanessian, *Total synthesis of Natural product: The chiral approach Vol.III* Pergamon Press 1983.
- W. D. Foye, T. L. Lemke, and D. A. Williams: *Principles of Medicinal Chemistry* (4<sup>th</sup> Edition)
- R. B. Siwerman: *Organic Chemistry of Drug Action and Design* (Academic press, 1993).

## CHM T 609: Advanced Heterocyclic Chemistry

Credits: Theory-03

Theory: 45 Hours

### Unit – 1: Introduction

Definition of heteroatom, Aromatic and non-aromatic heterocyclic compounds, Classification and nomenclature of heterocyclic compounds, important reactions with heterocyclic compounds i.e. oxidation, reduction and tertiary effect of Nitrogen in heterocyclic compound.

(9 Hours)

### Unit – 2: Non-Aromatic Heterocycles

Different types of strains, interactions and conformational aspects of non-aromatic heterocycles. Synthesis, reactivity and importance of the following ring systems: Aziridines, Oxiranes, Thiiranes, Oxaziridines, Azetidines, Oxetanes and Thietanes.

(9 Hours)

### Unit – 3: Five and Six Membered Heterocyclics with One Hetero Atom

Pyrrrole, Furan, Thiophene, Pyridine, Indole, Quinoline, Isoquinoline - Synthesis and reactions [Advanced synthetic methods are applied].

(9 Hours)

### Unit – 4: Five and Six Membered Heterocyclics with Two Hetero Atoms

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine, Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

(9 Hours)

### Unit – 5: Larger Ring and Other Heterocycles

Synthesis, structure, stability and reactivity of Azepines, Oxepines and Thiepines. Synthesis of Benzoazepines, Benzooxepines, Benzothiepines, Azocines and Azonines.

(9 Hours)

### Reference Books:

- T. Gilchrist: *Heterocyclic Chemistry*
- R. M. Acheson: *An Introduction to the Chemistry of Heterocyclic Compounds*
- J. A. Joule & K. Mills: *Heterocyclic Chemistry*
- A. Paquette: *Principles of Modern Heterocyclic Chemistry*
- J. A. Joule & Smith: *Heterocyclic Chemistry*
- A .R. Katritzky: *Handbook of Heterocyclic Chemistry*

## CHM T 610: Chemistry of Natural Products

Credits: Theory-03

Theory: 45 Hours

### Unit – 1: Alkaloid – I

Occurrence and isolation, biological role of alkaloids, General properties, nomenclature and classification of alkaloids on the basis of amino acid origin and present core structure. Isolation, properties and structural elucidation of quinine, Morphine (structure, synthesis, molecular rearrangement, stereochemistry and biogenesis).

(9 Hours)

### Unit – 2: Alkaloid – II

Structure and biological role of nicotine, cocaine, quinine, reserpine, vincristine, morphine, caffeine, papavarine, hyocimine. Strychnine and lysergic acid.

(9 Hours)

### Unit – 3: Steroid

Introduction, nomenclature of steroids, absolute configuration of steroid. Occurrence, isolation, structure elucidation and chemical properties of Cholesterol.

(9 Hours)

### Unit – 4: Terpenes

Secondary metabolites: Definition and examples; terpenes – isoprene rule; mono terpenes: structure of geraneol, limonene, alpha-pinene and camphor; sesquiterpenes: longfolene;

diterpenes: abietic acid, taxol. Structure determination of Citral and Camphor.

(9 Hours)

### Unit – 5: Vitamins

Introduction, chemical properties, structure elucidation of Vitamin A, Vitamin B, Ascorbic Acid and Vitamin D. Vitamin A and its role in vision. Biological role of Vitamin D, Ascorbic Acid, Vitamin A.

(9 Hours)

### Reference Books:

- I. L. Finar: *Organic Chemistry Vol. II*, 5th Edition
- S. V. Bhat, B. A. Nagaramgagi, M. Srikumar: *Chemistry of Natural Products*, Alpa Science International Ltd, 2005 by
- O. P. Agarwal: *Chemistry of Natural Products, Vol I & Vol II*, Goel publishing House, 1989
- J. R. Hanson: *Natural Products: The Secondary Metabolites*, Wiley-Vch, 1<sup>st</sup> Ed.; 2008.

## CHM T 611: Solid State Chemistry

Credits: Theory-03  
Theory: 45 Hours

### Unit – 1: Crystal Structure

Crystalline and amorphous solids; symmetry in crystals, basic crystal systems, space lattice and unit cell, Bravais lattice, miller indices, closed packed structure- hcp and ccp, packing efficiency, limiting radius ratio and shape of ionic crystal, description of solids; structure types Rock salt (NaCl), Zinc blende (ZnS), antiferite (Na<sub>2</sub>O), Rutile (TiO<sub>2</sub>), Wurzite (ZnS), CdCl<sub>2</sub>, nickel arsenide, CsCl, CdI<sub>2</sub>, Cs<sub>2</sub>O, perovskite ABO<sub>3</sub>, K<sub>2</sub>NiF<sub>4</sub>, spinels.

(9 Hours)

### Unit – 2: Point Groups

Symmetry operation and symmetry elements, Plane of symmetry, inversion centre, proper and improper axis of rotation, Product of symmetry operation, Relation among symmetry elements and symmetry operation, classification of symmetry, symmetry elements in octahedral and tetrahedral molecules, symmetry point group, representation of symmetry operation by matrices, reducible and irreducible representation, Character tables.

(9 Hours)

### Unit – 3: Space Groups

Thirty two point groups, Representation of point groups and selected examples like 222, mm2, mmm, 32 centrosymmetric and noncentrosymmetric point groups, space group: Triclinic P1, monoclinic C2, monoclinic C2/m, orthorhombic P222<sub>1</sub> orthorhombic F222, Tetragonal 14<sub>1</sub>, space group and crystal structure of SrTiO<sub>3</sub> and rutile structure of TiO<sub>2</sub>.

(9 Hours)

### Unit – 4: Structure and Properties of Advance Materials – I

Superconductors – (Ba,K)BiO<sub>3</sub>, Cuprates, LnFeAsO, MgB<sub>2</sub>, CaC<sub>6</sub>

CMR materials – La<sub>(1-x)</sub>Sr<sub>x</sub>MnO<sub>3</sub>

Ferriic compounds – BaTiO<sub>3</sub>, PbTiO<sub>3</sub>, Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub>, SrRuO<sub>3</sub>

Peizoelectric materials- PZT,

Photoluminescent materials – Lanthanide compounds

Porous materials – zeolites, AlPO, MeAlPO, SAPO.

(9 Hours)

### Unit – 5: Structure and Properties of Advance Materials – II

Organic-inorganic hybrid materials – MOF compounds

Ionic Conductors – NASICON, AgI, NaAl<sub>11</sub>O<sub>17</sub>

Thermoelectric materials – Na<sub>x</sub>CoO<sub>2</sub>, AgSbTe<sub>2</sub>, CoSb<sub>3</sub>, Y<sub>14</sub>MnSb<sub>11</sub>

Compounds for intercalation and redox reactions – LiCoO<sub>2</sub>, LiVS<sub>2</sub>, NASICON, Chevrel phases

(9 Hours)

### Reference Books:

- C. N. R. Rao and J. Gopalakrishnan: *New Direction in Solid State Chemistry*, Cambridge University Press, 1997.
- A. R. West: *Solid State Chemistry and Its Applications*, John Wiley & Sons, 1989.
- L. Smart and E. Moore: *Solid State Chemistry*, Chapman and Hall, 1992.

## CHM T 612: Advanced Synthetic Organic Chemistry

Credits: Theory-03

Theory: 45 Hours

### Unit – 1: Metal Mediated C-C and C-X Coupling Reactions

Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions. **C=C Formation Reactions:** Shapiro, Bamford-Stevens, McMurrey reactions, Julia Lythgoe olefination and Peterson's stereoselective olefination. Olefin metathesis by I<sup>st</sup> and II<sup>nd</sup> generation catalysts: Reaction mechanism and application in the synthesis of heterocycles.

(9 Hours)

### Unit– 2: Reagents of Phosphorous, Sulfur, Silicon and Boron

Phosphorous Sulfur, Silicon and Boron containing compounds-preparations and their uses in organic reactions.

(9 Hours)

### Unit – 3: Oxidation and Reduction

**Oxidation:** Oxidation of hydrocarbons (alkanes, aromatic hydrocarbons, alkenes), Oxidation of alcohols (Chromium reagents, Manganese reagents, Other metal and non-metal based oxidants), Oxidation of ketones (  $\alpha$ ,  $\beta$ -unsaturated ketones,  $\alpha$ -hydroxy ketones, Baeyer-Villiger oxidation of ketone)

**Reduction:** Catalytic hydrogenation, Reduction by dissolving metals, Reduction by hydride-transfer reagents (Derivatives of lithium aluminium hydride and sodiumborohydride, mixed lithium aluminium hydride-aluminium chloride reagent, DIBAL-H, NaBH<sub>3</sub>CN, sodium triacetoxyborohydride, Borane and derivatives, other methods of reductions).

(9 Hours)

### Unit – 4: Disconnection Approach, Umpolung Chemistry and Protection-Deprotection of Functional groups

Basic principles and terminology-Target molecule, FGI, Disconnection, Synthon, Reagent and Retro-synthetic approach. **One group C-C and C-X disconnection:** (disconnection of alcohols, alkenes, and carbonyl compounds). **Two group C-C & C-X disconnections:** 1,3 and 1,5 difunctionalised compounds,  $\alpha$ ,  $\beta$ , unsaturated carbonyl compounds, control in carbonyl condensation, synthesis of 3,4,5 and 6 membered rings in organic synthesis. Diels-Alder reaction, connection in retro synthesis. Umpolung in organic synthesis. Protection and deprotection for functional groups as hydroxyl, amino, carboxylic and carbonyl.

(9 Hours)

### Unit – 5: Some Important Organic Reactions

**Selective Stereoselective Organic Reactions with Alkenes:** Sharpless Asymmetric Epoxidation, Asymmetric Aziridination, Dihydroxylation, Amino-hydroxylation Reactions, Oxidative cleavages of alkenes.

**Green Chemistry,** Supramolecular chemistry (Crown ether, Cyclodextrin and Clalixerins) and multicomponent reactions (Ugi, Passerini, Biginelli, Hantzsch reactions).

**Chemistry of Aliphatic and Aromatic Heterocyclic Compounds:** Epoxide, Aziridine, Azitidine, Oxetane, Pyrrole, Furan, Thiophene, Pyridine, Indole, Quinoline, Isoquinoline - Synthesis and reactions.

(9 Hours)

### References Books:

- B. F. G. Johnson: *Transition Metal Cluster*, Wiley, 1980.
- R. H. Crabtree: *The Organometallic Chemistry of the Transition Metals*, Wiley-Interscience, 2005.
- G. Wilkinson, F. G. A. Stone, and E. Abel: *Comprehensive Organometallic Chemistry*, Peramon, 1980.
- I. Fleming: *Frontier Orbitals and Organic Chemical Reactions*, Wiley, 1976.
- B. B. Woodward and Hoffman: *Conservation of Orbital Symmetry*, Verlag Chemie Academic Press, 1971.
- S. Warren: *Organic Synthesis: The Disconnection Approach*, John Wiley & Sons (Asia) Pte. Ltd., 2007
- W. Carruthers and I. Coldham: *Modern Methods of Organic Synthesis*, Fourth Ed. Cambridge University Press.
- T. L. Gilchrist: *Heterocyclic Chemistry*, Pearson Education, 3rd Ed. 2007

## EVALUATION & DISTRIBUTION OF MARKS

**(1) Continuous Internal Assessment (CIA):** Forty (40) marks

- (a) 1<sup>st</sup> Mid-Semester Examination: Maximum Marks 10  
Duration of Examination: One Hour  
Pattern of Question Paper:  
Five (05) Objective Type Questions; each carrying one (1) mark  
One (01) Short Answer Type Question of five (05) marks
- (b) 2<sup>nd</sup> Mid-Semester: Maximum Marks 10 (as described above)
- (c) Assignment (minimum one): Maximum 15 Marks
- (d) Regularity in the Class: Maximum five (05) Marks:  
Award of marks based on attendance will be determined as below:

| Attendance    | Marks   |
|---------------|---------|
| 90% and above | 5 Marks |
| 85 to 89.9%   | 4 Marks |
| 80 to 84.9%   | 3 Marks |
| 76 to 79.9%   | 2 Marks |
| 75 to 75.9%   | 1 Mark  |
| Below 75%     | Zero    |

**Note:** Total Marks of CIE will be 40 (i.e., 10+10+15+5). A candidate must have to secure minimum 50% marks (i.e., 20 out of 40 marks). Failing so, s/he shall not be allowed to appear in End Semester Examination.

Marks for two mid-semester examinations could either be awarded as aggregate scored by the candidate in the two exams or as best of two. The department may adopt suitable model.

**(2) End Semester Examination (ESE)**

- (a) Theory Paper: Maximum Marks: 60 (Sixty)  
Duration of Examination-Three Hours  
Question Paper Pattern: The paper will be set so to cover all units/sections of the syllabus as below:

| Type   | Total No.                        | No. of questions to be answered | Marks for Each Question | Total Marks |
|--|----------------------------------|---------------------------------|-------------------------|-------------|
| Long Answer Type Questions (one out of two questions from each unit) | 05 (one question from each unit) | 5 (from all five questions)     | 12                      | 60          |
| <b>Total</b>   |                                  |                                 |                         | <b>60</b>   |

- (b) Practical Examination:  
Duration of Examination: Four - Six Hours  
Question Paper Pattern –

|                    |                        |           |
|--------------------|------------------------|-----------|
| Q.1.<br>Experiment | Principle/ Theory      | 10        |
|                    | Procedure              | 10        |
|                    | Results and discussion | 10        |
| Q.2                | Viva-voce              | 10        |
| Q.3                | Record/ File           | 10        |
|                    | <b>Total</b>           | <b>50</b> |

(3) Total marks of each question paper will be 100 (hundred) for theory paper [i.e., 60 (ESE) + 40 (CIA)] and 50 (fifty) for practical paper (Grand Total: **150, Hundred-Fifty**), irrespective of their credits.

**(4) Attendance**

A candidate shall only be eligible to appear in the end-semester examination if s/he has secured a minimum of 75% attendance as prescribed in the university ordinance.

**(5) Grading**

Each course shall be graded (refer table below) on the basis of marks obtained, on scaled marks of 100, during a semester. There shall be absolute grading where mark obtained (out of 100) by a student in a course is converted to a Grade on a 10-point scale.

**Table:** Showing marks to grade conversion