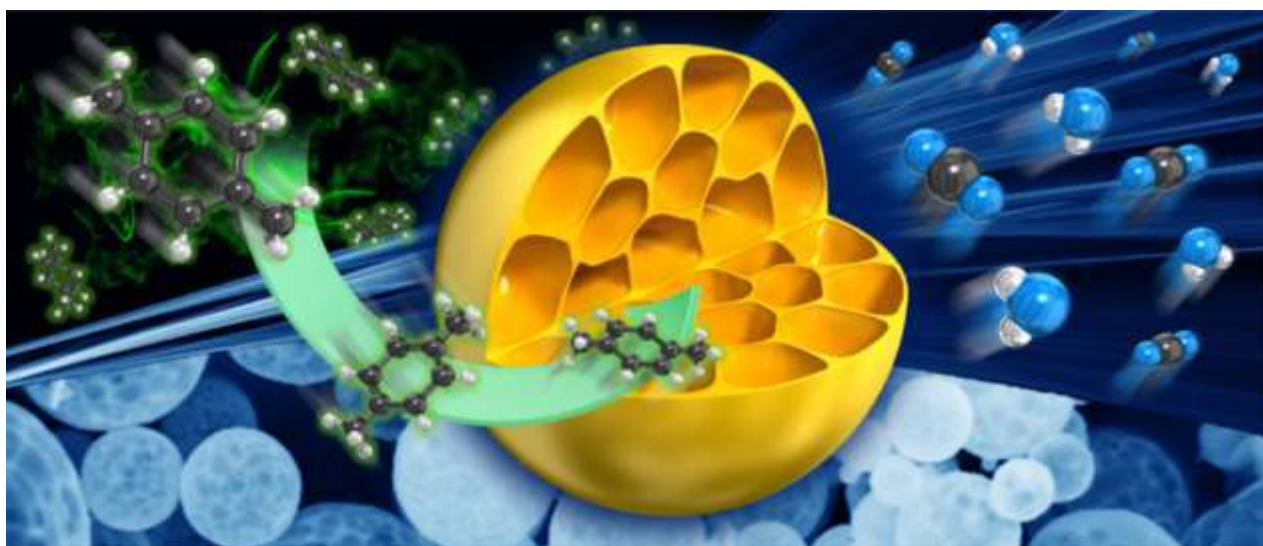


**M.Sc. Chemistry**  
**(CBCS)**  
**SYLLABUS**



Department of Chemistry  
Central University of Tamil Nadu  
Thiruvarur 610 005

2018

## Programme Structure

<b>Duration</b>	:	4 semesters
<b>Intake</b>	:	16

The five year program is spread into ten semesters where in first four semesters are designed for broad subject based understanding. Later six semesters will have increased focus on chemistry.

The subject courses in the early stage of iM.Sc programme are simplified and of basic level that bolsters the inter-disciplinary way of learning. The third and subsequent year courses have been designed on advanced theories in chemistry with emphasis on concurrent modern laboratory techniques. Further the iM.Sc (Chemistry) programme has been included with experiments that provide exhaustive hands on experience on various sophisticated instruments, experimental techniques to enable the students secure jobs in corporate. The final semester is dedicated to specialization within the subject with research level training.

The rules and regulations of Choice Based Credit System (CBCS) are applicable to this program. Generally, a student takes ten semesters to complete the program. The courses offered under CBCS, has certain credit number (2, 3 or 4). Core requirements of the programs are clearly defined. In the first two years of the program, a student has common course load with students from other departments. From fifth semester onwards, students will have courses more tuned towards chemistry. Apart from courses offered by the Department of Chemistry, student shall take prescribed number of elective courses either from parent department or from other departments

**CENTRAL UNIVERSITY OF TAMIL NADU, THIRUVARUR**  
**M.Sc. CHEMISTRY SYLLABUS CREDIT DISTRIBUTION**

Semester	Title of the Course	Nature of the course	Credit
1	Solid State, Main Group and Coordination Chemistry	T	4
1	Physical Organic Chemistry & Aromatic Compounds	T	4
1	Chemical Kinetics & Group Theory	T	4
1	*****Subject Selective Elective*****	E	4
1	Advanced Organic Chemistry Laboratory	P	4
2	Advanced Organometallic & Bioinorganic Chemistry	T	4
2	Organic Photochemistry & Rearrangements	T	4
2	Advanced Quantum Chemistry & Molecular Spectroscopy	T	4
2	Physical Methods in Chemistry I	T	4
2	Advanced Physical Chemistry Laboratory	P	4
3	Physical methods in Chemistry II	T	4
3	Reagents & Synthetic Strategies in Organic Chemistry	T	4
3	Thermodynamics (Classical/statistical) & Electrochemistry	T	4
3	*****Subject Selective Elective*****	E	4
3	Advanced Inorganic Chemistry Laboratory	P	4
4	Research Project	P	12
	TOTAL		72

**Semester I**  
**Solid State, Main Group and Coordination Chemistry**

**Credit: 4**

**Theory**

**Objectives:**

To introduce the concept of solid state chemistry, structural diversity of the main group elements, and advanced level of coordination chemistry and its multitudes of applications.

**Learning Outcomes:**

Ensures the students to gain the concept of solid state chemistry, understand the structure and properties relationship of the main group elements, coordination chemistry and reaction mechanisms.

**Synthesis and modification of inorganic solids:** Structures of ionic crystals – AX and AX<sub>2</sub> type crystal structures – layer structures - lattice energy - Born-Landé, Born-Mayer and Kapustinskii equations – Derivations and applications –Review of defects in ionic solids - Thermodynamic effects of defects. Band theory, n- and p- type semiconductors and superconductors. Reactions in solid state - diffusion, diffusion coefficient, diffusion mechanisms, vacancy and interstitial diffusion, thermal decomposition of solids -Type I and Type II reactions. Phase Transitions - classification of phase transitions-first and second order phase transitions, Martensitic transformations, order-disorder transitions. Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods. Molecular material and fullerenes, molecular materials & chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystals.

**The Chemistry of the Main Group Elements:** Inorganic Rings, chains, and cages Catenation and Heterocatenation, Heterocyclic ring system- Borazines, Phosphazines- Monomer and Polymer, S-N ring compounds, Homocyclic rings of S, Se and Te. Silicate minerals, Isopolyanions, Boranes: boron cage compounds-closo, nido, arachno, carboranes; cage compounds of S and P. Metal cluster: metal-metal bonding and reactivity of di-, tri- and polynuclear clusters.

**Coordination Chemistry II:** Recapitulation of Crystal field theory - splitting of d-orbitals under various geometries - Limitations of CFT – Ligand field Theory - MO theory – sigma – and pi-bonding in complexes and evidences for  $\pi$ -bonding – nephelauxetic effect – angular overlap model. Studies of coordination compounds in solution – detection of complex formation in solution – Stability constants – stepwise and overall formation constants – simple methods (Potentiometric, pH metric and photometric methods) of determining the formation constants - factors affecting stability – Irving-William series -statistical and chelate effects – forced configurations.

**Coordination Chemistry-III:** Reaction Mechanism: Kinetics and mechanism of reactions in solution – labile and inert complexes – ligand displacement reactions in octahedral and square planar complexes – acid hydrolysis, base hydrolysis and anation reactions – trans effect – theory and applications. Electron transfer reactions – complementary and non-complementary types – inner sphere and outer sphere processes – Excited state outer sphere electron transfer reactions - isomerisation and racemisation reactions of complexes –

reactions of four and six-coordinate complexes – interconversion between stereoisomers.

### **Prescribed Books**

1. Huheey J. E., Keiter E. A. and Keiter R. L. and Medhi O. K., Inorganic Chemistry - Principles of Structure and Reactivity, 4th edition, Pearson Education, **2006**.
2. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 8th edition, **2009**.
3. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd edition, John Wiley & Sons, **2010**.
4. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 3rd ed. Wiley-Eastern Company, New Delhi, **1990**.
5. Azaroff, L.V., Introduction to Solids, McGraw hill, New York. **1960**.
6. West, A. R., Solid State Chemistry and Its Applications, John Wiley & Sons, **1984**.
7. Chakrabarty, K., Solid State Chemistry, New Age Publishers, **1996**.
8. Keer, H. V., Principles of the Solid State, Wiley Eastern Limited, **1993**.
9. D.M. Adams, Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry, Wiley, **1974**.
10. C.N.R. Rao, K.J. Rao, Phase Transitions in Solids, McGraw Hill, **2010**.
11. A.Earnshaw, Introduction to Magnetochemistry, Academic Press, **1968**.

### **Reference Books**

1. Day, M. C., and Selbin, J., Theoretical Inorganic Chemistry, Affiliated East West Press Pvt. Ltd. 2nd edition, **1985**.
2. Kettle, S. F. A., Physical Inorganic Chemistry – A Coordination Chemistry Approach, Spectrum Academic Publishers, Oxford University Press, **1996**.
3. Basolo, F., and Pearson, R. G., Mechanism of Inorganic Reactions, John Wiley, New York, **1967**.
4. Miessler, G. L., and Tarr, D. A., Inorganic Chemistry, 3rd edition, Pearson, **2004**. Housecraft, C. E., and Alan G. Sharpe, Inorganic Chemistry, 4th edition, Pearson, **2012**.
5. Purcell, K. F., and Kotz, J. C., Inorganic Chemistry, Cengage Learning, **2012**. Day Jr, M. C., and Selbin, J., Theoretical Inorganic Chemistry, Literary Licensing, LC, **2012**.
6. Wilkinson, G., Gillars, R. D., and McCleverty, J. A., Comprehensive Co-ordination Chemistry, Pergamon Press, **1987**.
7. Wulfborg, G., Inorganic Chemistry, University Science Books, **2000**.
8. Adam, D.M. Inorganic Solids: An introduction to concepts in solid-state structural chemistry. John Wiley & Sons, **1974**.
9. Rodger, G.E. Inorganic and Solid State Chemistry, Cengage Learning India, Edition, **2002**.

**Semester I**  
**Physical Organic Chemistry & Aromatic Compounds**

**Credit: 4**

**Theory**

**Specific objectives:**

To introduce the advanced level concepts in stereochemistry, aromaticity, heterocyclic compounds and physical organic chemistry.

**Learning outcomes:**

Ensures the students to understand, acquire knowledge on topicity, asymmetric synthesis, determining the reaction mechanisms by different methods, criteria for aromaticity in non benzenoid molecules and other advanced polycyclic aromatics and the nomenclature and reactions of complex heterocyclic.

**Advanced Stereochemistry:** Configuration - conformation of cycloalkanes, conformation and reactivity - stereochemistry of allenes, spiranes, biphenyls, molecules with chiral planes, Topicity stereoselective and stereospecific reactions - enantioselective reactions - double stereo differentiation, asymmetric synthesis, chiral auxiliaries, chiral catalysts and reagents.

**Physical organic chemistry:** Thermodynamic stability – general relationship between thermodynamic stability and reaction rates – electronic substituent effects on reaction intermediates – kinetic isotope effects – linear free energy relationships – principles of microscopic reversibility – substituent effects – solvent and solvent effects – methods of determination of reaction mechanism.

**Aromaticity:** Criteria of aromaticity - Craig's rule – non-benzenoid aromatic compounds – anti-aromaticity, homoaromaticity – fused-ring systems –hetero aromatic systems. Nucleophilic aromatic substitution reactions – VNS - transition metal- catalyzed aromatic substitution reactions – aromatic substitution reactions involving radical intermediates.

**Advanced Heterocycles:** Nomenclature, heterocyclics with two hetero atoms – fused five and six membered heterocyclics – preparation and reactions of indole, quinoline, isoquinoline and carbozole.

**Prescribed books:**

1. Carey, F.A., Sundberg, R.J., Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edn, Springer, **2007**.
2. Carey, F.A., Sundberg, R.J., Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th edn, Springer, **2007**
3. Nasipuri, D., Stereochemistry of Organic Compounds: Principles and Applications 4th edn, New Academic Science Publisher, **2012**.
4. Eliel, E. L., and Wilen, S. H. Stereochemistry of Organic Compounds, Wiley, **1994**.
5. Joule, J.A., Mills, K, Heterocyclic Chemistry, 5th edn, Wiley-Blackwell, 2010.
6. Bansal, R. K., Heterocyclic Chemistry, 5th edn, New Age International Private Limited, **2017**

## Reference books

1. Morrison, R.T., Boyd, R.N. Bhattacharjee, S. K., Organic Chemistry, 7th edn, Pearson Education, **2010**.
2. Pine, S. H., Organic Chemistry, 5th edn, Tata McGraw Hill, **2008**.
3. Carruthers, W., Coldham, I., Modern Methods of Organic Synthesis, 4th edn, Cambridge University Press, **2015**.
4. Smith M. B., March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th edn, Wiley, **2015**
5. Finar, I.L. Organic Chemistry, Vol I, 6th edn, Pearson Education, **2002**
6. Sykes, P. A Guidebook to Mechanism in Organic Chemistry, 6th edn, Pearson Education, **2003**.
7. Kalsi, P. S., Stereochemistry: Conformation and Mechanism, 9th edn, New Age International Private Limited, **2017**
8. Katritzky, A. R., Ramsden, C. A., Joule, J. A., Zhdankin, V. V., Handbook of Heterocyclic Chemistry, 3rd edn, Elsevier, **2010**.
9. Anslyn, E. V., Dougherty, D. A., Modern Physical Organic Chemistry, University Science Books, **2005**

### Semester I

### Chemical Kinetics & Group Theory

Credit: 4

Theory

#### Course objective

- To introduce the essential concepts of chemical kinetics; important postulates and theories.
- To familiarize about the widely applicable enzyme catalysis and its mechanism.
- To predict the kinetics of Rice – Herzfeld mechanisms and explosive reactions.
- To give an overview of Group theory, Symmetries, Optical Activity, Dipole Moment and Irreducible Representations.
- To apply Applications of symmetry concepts in Spectroscopies and Chemical Bonding.

#### Course outcome

After successful completion of this course, the students will able

- To use various experimental techniques to determine the kinetics of chemical reactions.
- To determine the overall symmetry of any small and medium-sized molecule and apply concept of point group and GOT to study their chemical properties.

### Chemical Kinetics

Reaction rates and order of reactions, determination of order of reactions, complex reactions, reversible, consecutive and concurrent reactions. Reactions of variable order- steady state treatment, free radical reactions-the Rice Herzfeld Mechanism.

Fast reactions: relaxation, Flow and Shock methods, Molecular beam methods Flash photolysis. Introduction to femtochemistry

Theories of reaction rates: Arrhenius equation, Collision cross section and reaction cross section. -steric factor, potential energy surfaces, Thermodynamic formulations of Collision

& Transition state theories Comparative study of the theories of reaction rates. Thermodynamic treatment of Reaction rates, Effect of pressure on velocity of gas reactions. Molecular Reaction Dynamics: Heterogeneous catalysis: Unimolecular and bimolecular surface reactions, Langmuir-Hinshelwood and Langmuir-Rideal mechanism-ARRT of surface reactions,

Enzyme catalysis: Michelis-Menten equation, effect of pH and temperature on enzyme catalysis.

Eley-Rideal and Hinshelwood mechanisms, Lindemann-Hinshelwood mechanism, qualitative idea of RRKM theory, chain reactions, steady state treatment (kinetics of  $\text{H}_2\text{-Cl}_2$  and  $\text{H}_2\text{Br}_2$  reactions), Rice – Herzfeld mechanism, Explosive Reactions  $\text{H}_2\text{-O}_2$  (Semenov-Hinshelwood)

### **Group Theory:**

Symmetry: Fundamentals Concept of Symmetry, Matrix representation of symmetry operations. concepts of groups, molecular point groups, representation of groups, matrix representation of symmetry operations, reducible and irreducible representations, Symmetry criterion of optical activity, symmetry restrictions on dipole moment.

Great Orthogonality Theorem: Interpretation of character tables. Determination of symmetry species for translations and rotations.

Vibrational spectra: transition moment integral, vanishing of integrals, symmetry aspects of molecular vibrations, vibrations of polyatomic molecules-selection rules for vibrational absorption. Symmetry of normal modes of  $\text{H}_2\text{O}$ ,  $\text{C}_2\text{H}_4$ , Trans- $\text{N}_2\text{F}_2$ ,  $\text{CHCl}_3$  and  $\text{NH}_3$  using Cartesian coordinates and internal coordinates.

### **Applications in Spectroscopy**

- I. Complementary nature of IR and Raman spectra-determination of the IR and Raman active vibrational modes
- II. Electronic spectra: selection rules for electronic transition, electronic transitions simple aldehydes

### **Applications in chemical bonding**

- I. Transformation of atomic orbitals- Symmetry adapted linear combinations (SALC), Construction of hybrid orbitals for  $\text{AB}_3$ (planar),  $\text{AB}_4$ (Td),  $\text{AB}_5$ ( $\text{D}_{3h}$ ) and  $\text{AB}_6$ (Oh) type of molecules
- II. Ligand field theory-splitting of d orbitals in different environments using group theoretical considerations
- III. MO diagram for water and ammonia, method of descending symmetry

### **Reference Books**

1. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, New York, **1988**
2. F. Daniels and R. A. Alberty, Physical Chemistry, 8h Edition, Wiley, New York, **1994**
3. P. W. Atkins, Physical Chemistry 8th Edn., Wiley, New York, **2006**

4. J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, **2000**.
5. K.J. Laidler, Chemical kinetics, 3rd Edn. Harper & Row, **1987**.
6. C. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International, **2005**.
7. D.A. McQuarrie, J. D. Simon, Physical chemistry: A Molecular Approach, University Science Books, **1997**
8. F. A. Cotton: Chemical Applications of Group Theory, Wiley Eastern, **1985**.
9. P. K Ghosh and P. K Shukla: Atomic Electronic Structure, Prentice Hall of India, **1994**.
10. V. Ramakrishnan and M. S. Gopinathan: Group Theory in chemistry, Vishal Publication, **1986**.
11. D. M. Bishop, Group theory and Chemistry, Dover, **1989**.

**Semester I**  
**Advanced Organic Chemistry Laboratory**

**Credit: 4**

**Practical**

**Specific objectives:**

To introduce the experimental aspects of advanced organic chemistry involving multistep synthesis, qualitative and quantitative analysis of organic compounds.

**Learning outcomes:**

Ensures the students to understand, acquire knowledge and have hands on experience in multistep organic synthesis and analysis by using spectroscopic techniques. Separation techniques and functional group analysis.

1. Multistep organic synthesis (any four) - conventional synthesis - microwave assisted synthesis - photochemical reactions. Purification of the compounds using column chromatography and characterization of the compounds using spectroscopic techniques.
2. Qualitative Analysis: Separation and analysis of organic mixture containing two components and preparation of suitable derivatives (at least four compounds).
3. Estimation of organic compounds:
  - a) Estimation of phenol and aniline - volumetric method.
  - b) Estimation of glucose by Betrands method.
  - c) Estimation of methyl ketone – iodimetric method
  - d) Differentiation between a reducing and a nonreducing sugar.
  - e) Determination of iodine and saponification value of an oil sample.

## Prescribed Books

1. Vogel, A. I., Elementary Practical Organic Chemistry: Small Scale Preparations, Qualitative Organic Analysis, Quantitative Organic Analysis, Pearson Education, **2011**.
2. Ahluwalia, V.K., Aggarwal, R. Comprehensive Practical Organic Chemistry, Universities Press, **2004**
3. Bansal R. K., Laboratory Manual in Organic Chemistry, New Age International Pvt. Ltd Publishers, **2009**.
4. Mann, F.G., Saunders, B.C. Practical Organic Chemistry, 4th edn, Pearson Education India, **2009**
5. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J., Smith, P.W.G., Vogel's Practical Organic Chemistry, 5th edn, Pearson Education Ltd, **1996**.

## Reference Books

1. Leonard, J., Lygo, B., Procter, G., Advanced Practical Organic Chemistry, 3rd edn, CRC Press, **2013**.
2. Cranwell, P. B., Harwood, L. M., Moody, C. J., Experimental Organic Chemistry, 3rd edn, Wiley-Blackwell, **2017**.

## Semester II Advanced Organometallic & Bioinorganic Chemistry

Credit: 4

Theory

### Specific objectives:

To the concepts of organometallics, bonding, structure, reaction mechanism and catalysis and to introduce the principles of bioinorganic chemistry and

### Learning outcomes:

Upon successful completion of this course, the student should be able to:

- Ensures the students to understand, acquire knowledge on ligands and fluxional molecules, different organic ligands and metal complexes, reaction mechanism and catalysis.
- Understand the concepts of Bioinorganic Chemistry.
- Understand the function and transport of Alkali and Alkaline earth metals in the biological systems.
- Describe the important roles of metal ions in metalloproteins/metalloenzymes.
- Identify the appropriate analytical techniques that are useful in characterizing transition-metal coordination in biological molecules.
- Understand the importance of metal ions in medicine.

**Structure and bonding in organometallics:** 16/18-Electron rule - metal carbonyls – bonding –spectra – metal alkyls, aryls, hydrides and dihydrogen complexes - ligands – metallocenes - electronic structure and bonding in ferrocene - synthesis, physical and spectroscopic properties of metallocenes – fluxional molecules.  $\sigma$ -bonded ligands: metal-phosphines / metal- nitrosyls: structures, reactivity and bonding. Carbenes: N-heterocyclic

carbenes, Fischer carbenes, Schrock carbenes, carbynes. Isolobal analogy, metal-metal bond, transition metal clusters. Quintuple bond.

**Reaction mechanism and catalysis:** oxidative addition, reductive elimination, insertion, hydride elimination, abstraction; hydrogenation of olefins, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, Isomerization reactions, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation, carbonylation, and CH functionalization reactions.

**Bioinorganic Chemistry II:** Metalloporphyrins/Metalloenzymes

**Metals at the Center of Photosynthesis:** Primary Processes in Photosynthesis – Photosystems I and II - Light Absorption (Energy Acquisition) – Exciton transport (Direct Energy Transfer) – Charge separation and electron transport – Manganese catalyzed oxidation of water to O<sub>2</sub>.

Dioxygen transport and storage - hemoglobin and myoglobin: electronic and spatial structures - hemerythrin and hemocyanine – synthetic Oxygen carriers, model systems - blue copper proteins (Cu) - iron-sulfur proteins (Fe) - cytochromes electron transport chain - carbon monoxide poisoning - iron enzymes - peroxidase, catalase and cytochrome P-450, copper enzymes - superoxide dismutase, carboxypeptidase, carbonicanhydrase, vitamin B<sub>12</sub> and B<sub>12</sub> coenzymes, nitrogen fixation. Medicinal bioinorganic chemistry: platinum complexes in cancer therapy – cis-platin and its mode of action – metal toxicity.

**Magnetic properties:**Types of magnetism – Dia –para – ferro and antiferro magnetism. Magnetic properties of free ions – first order Zeeman effect – Second order Zeeman effect – states  $KT$  – states  $\ll KT$ . Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature dependent and temperature independent paramagnetism - Magnetic properties of lanthanides and actinides. Spin crossover in coordination compounds.

### Prescribed Books

1. Powell, P., Principles of Organometallic Chemistry, 2nd ed., Springer, 1998.  
Purcell, K. F., and Kotz, J. C., Inorganic Chemistry, Saunders Golden Sunburst Series, W.B. Saunders Company, Philadelphia, 1977.
2. Huheey, J. E., Keiter, E. A. and Keiter, R. L. and Medhi, O. K., Inorganic Chemistry - Principles of Structure and Reactivity, 4th edition, Pearson Education, 2006.
3. Mehrotra, R. C., and Singh, A., Organometallic Chemistry, a Unified Approach, New Age International, 2006.
4. Crabtree, R. H., Organometallic Chemistry of the Transition Metals, Wiley, New York, 1988.  
Gupta, B. D., and Elias, Anil. J., Basic Organometallic Chemistry: Concepts, Syntheses, and Applications of Transition Metals, 1st edition, Universities Press, CRC Press, 2010.
5. Lippard, S. J., and Berg, J. M., Principles of Bioinorganic Chemistry, Panima Publishing Company, New Delhi, 1997.

6. Kaim W., and Schewederski, B., *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*, John Wiley & Sons, New York, USA, 2013.
7. Bertini, I., Gray, H. B., Lippard, S. J. and Valentine, J. S., *Bioinorganic Chemistry*, 1st South Asia edition, Viva books Pvt. Ltd., 2007.
8. S. P. Banerjee, *Advanced Inorganic Chemistry*, Arunabha Sen, Books and Allied (P) LTD. Volume II, 2015.

### Reference Books

1. Elschenbroich, C., and Salzer, A., *Organometallics: A Concise Introduction*, 3rd edition, 1999.
2. Greenwood, N. N., and Earnshaw, A., *Chemistry of the Elements*, 2nd edition, Elsevier, 2005.
3. Jolly, W. L., *Modern Inorganic Chemistry*, McGraw Hill, New York, 2nd Edition, 1991.
4. Kegley, S. E., and Pinhas, A. R., *Problems and Solutions in Organometallic Chemistry*, University Science Books, Oxford University Press, 1986.
5. Douglas, B., McDaniel, D. H., and Alexander, J. J., *Concepts and Models of Inorganic Chemistry*, 2nd edition, John Wiley & sons, New York, 2006.
6. Bochmann, M., *Organometallics 1: Complexes with transition metal-carbon  $\sigma$ -bonds*; Oxford Chemistry Primers Series, No. 13 Oxford Chemistry Primers Series, No.12, 1994.; Bochmann, M., *Organometallics 2: Complexes with transition metal carbon  $\pi$  bonds*, 1994.
7. Collman, J. P., Hegedus, L. S., Norton, J. R. and Finke, R. G., *Principles and Applications of Organotransition Metal Chemistry*, University Science Books. Mill Valley, California, 1987.
8. R. H. Crabtree, *Organometallic Chemistry of the Transition Metals*, Wiley, New York, 1988.
9. W. Parkins and R. C. Poller, *An Introduction to Organometallic Chemistry*
10. Haiduc and J. J. Zuckerman, *Basic Organometallic Chemistry*
11. R. Hoffmann, *Angew. Chem. Int. Ed.*, Engl. 21, 711-800 1982.
12. BD Gupta and Anil J. Elias, *Basic Organometallic Chemistry: Concepts, Syntheses, and Applications of Transition Metals*, 1st edition, Universities Press, CRC Press, 2010.
13. Cotton, F. A., Wilkinson, G., Carlos A. Murillo, Manfred Bochmann, *Advanced Inorganic Chemistry*, 6th ed., A Wiley - Interscience Publication, John -Wiley & Sons, USA, 2007. *Chem. Education*, 62, No. 11, *Bioinorganic Chemistry*, State of the Art. 1985.
14. Eichorn, G. L., *Inorganic Biochemistry*, Volumes 1 & 2, 2nd ed., Elsevier Scientific Publishing Company, New York, 1973.
15. Atkins, P., Overton, T., Rourke, J., Weller M., and Armstrong, F., *Inorganic Chemistry*, 5th edition, Oxford University Press, 2010.

**Semester II**  
**Organic Photochemistry & Rearrangements**

Credit: 4

Theory

**Specific objectives:**

To introduce the concepts of photochemistry, pericyclics, rearrangements and name reactions.

**Learning outcomes:**

Ensures the students to understand, acquire knowledge on pericyclic reactions, organic photochemistry, molecular rearrangement and name reactions and their further applications in organic synthesis.

**Pericyclic Reactions:** Pericyclic reactions – orbital correlation diagram – FMO. Diels-Alder reactions – 1,3-dipolar cycloaddition reactions – [2+2] cycloadditions and related reactions leading to cyclobutanes – [3,3] and [2,3]-sigmatropic rearrangements – unimolecular thermal elimination reactions.

**Organic photochemistry:** Photochemistry of alkenes, dienes and polyenes – photochemistry of carbonyl compounds – photoreductions, photooxidations and photorearrangement reactions - photochemistry of aromatic compounds.

**Molecular Rearrangements:** Applications of molecular rearrangement reactions in the synthesis of complex organic molecules and natural products.

**Selected name reactions in organic synthesis:** Julia olefination; Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction and Ugi reaction, Nazarov cyclization, Robinson annulation; McMurray reaction; Darzens reaction; Mitsunobu reaction; Dotz reaction;

**Prescribed books**

1. Carey, F. A., Sundberg, R. J., Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th edn, Springer, 2007.
2. Fleming, I., Pericyclic Reactions, 2nd edn, Oxford University Press, Oxford, 2015.
3. Sankararaman, S., Pericyclic Reactions - Applications and Theory, Wiley – VCH, 2005.
4. Turro , N. J., Scaiano, J. C., and Ramamurthy, V., Modern Molecular Photochemistry of Organic Molecules, University Science Books, 2010
5. Sanyal and Sanyal, Reactions, Rearrangements and Reagents, 4th edn, Bharati Bhawan Publishers and Distributors; 2003
6. Singh, J., Photochemistry and Pericyclic Reactions, 3rd edn, New Age International Publishers, 2012.

**Reference books**

1. Morrison, R.T., Boyd, R.N. Bhattacharjee, S. K., Organic Chemistry, 7th edn, Pearson Education, 2010.

- Pine, S. H., Organic Chemistry, 5th edn, Tata McGraw Hill, 2008.
- Smith M. B., March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th edn, Wiley, 2015
- Finar, I.L. Organic Chemistry, Vol I, 6th edn, Pearson Education, 2002
- Finar, I.L. Organic Chemistry, Vol II, 5th edn, Pearson Education India, 2002
- Sykes, P. A Guidebook to Mechanism in Organic Chemistry, 6th edn, Pearson Education, 2003
- Mukherjee, S.M., Singh, S.P., Reaction Mechanism in Organic Chemistry, Trinity Press, 2014.
- Lowry, T. H., Richardson, K. S., Mechanism and Theory in Organic Chemistry, 3rd edn, Addison – Wesley Longman Inc., 1998.
- Li, J. J., Corey, E. J., Name Reactions for Homologation, Part 1, Wiley-Blackwell, 2009
- Mundy, B. P., Ellerd, M G., Favaloro Jr. F. G., Name Reactions and Reagents in Organic Synthesis, 2nd edn, Wiley-Blackwell, 2005
- Carruthers, W., Coldham, I., Modern Methods of Organic Synthesis, 4th edn, Cambridge University Press, 2015.

## Semester II Quantum Chemistry & Molecular Spectroscopy

**Credit: 4**

**Theory**

**Course objective:**

- To solve Schrodinger equation for the most significant and elementary molecules using basic perturbation-variation principles and advanced VB-MO theories.
- To use the concept of LCAO to hybridization and directed bonding in polyatomic molecules.
- To introduce pulse sequences in magnetic resonance spectroscopy to avoid complexity in spectroscopy.
- To explain the basic principles and components of advanced molecular spectroscopy tools.

**Course outcome:**

After successful completion of this course, the students will able

- To understand recent computational chemistry and spectroscopic problems.
- Stepping stone to theoretical/Molecular spectroscopy/computational chemistry research

### Quantum Chemistry II

*Translational motion:* free particle in one-dimension, particle in a 1-D box with infinite & finite potential walls, tunneling, particle in a 3-D box. Nonplanar rigid rotor (or particle on a sphere)- separation of variables, the phi and the theta equations and their solutions, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms) - polar diagrams of spherical harmonics.

**Vibrational motion:** 1-D harmonic oscillator (complete treatment), Hermite equation (solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features, Harmonic oscillator model and molecular vibrations.

Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates: separation of Variables-R, theta and phi equations and their solutions, wave functions and energies of hydrogen-like atoms. Orbitals-radial functions, radial distribution functions, angular functions and their plots. The postulate of spin by Uhlenbeck and Goudsmith, discovery of Spin-Stern Gerlach experiment. Spin orbitals-construction of spin orbitals from orbitals and spin functions.

Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta ( $L_x$ ,  $L_y$ ,  $L_z$  and  $L^2$ )-commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators  $L_z$  and  $L^2$ . Ladder operator method for angular momentum. Space quantization.

Schrödinger equation for Helium atom. Perturbation theory, Variational methods, Hartree-Fock equations, Self-consistent field methods for solving Hartree-Fock equations, Born-Oppenheimer approximation-molecular Hamiltonian operators, Valence bond treatment for chemical bonding in molecules, molecular orbitals, molecular orbital theory for different diatomic molecular systems, photoelectron spectra, SCF-LCAO-MO wave functions, electronic states of diatomic molecules, sp, sp<sup>2</sup> and sp<sup>3</sup> hybrid orbitals, molecular term symbols, Hückel molecular orbitals, bonding in polyatomic molecules.

**EMR & Origin of spectra:** Nature of EMR, Interaction of EMR with matter, Natural line width and intensity of spectral lines, Classical and quantum chemical approach to absorption of radiation by molecules. Energy levels in molecules. Born Oppenheimer approximation, Population of energy levels.

### **Optical Spectroscopy**

**Microwave spectroscopy:** Molecular classification and Rotation spectra, Diatomic and polyatomic molecules. Application of Rotation spectra (Bond length, Isotopic mass, dipole moment, isotopic abundance), Non-rigidity of rotor.

**Vibrational spectroscopy:** Vibrational spectra of diatomics & SHO; anharmonicity & Morse potential; Vibration-rotational spectra of diatomics, polyatomic molecules-P,Q,R branches, Dispersive IR & FTIR, Vibration spectra of polyatomic molecules. Normal modes of vibrations of polyatomic molecules, Coupling of rotation and vibration, Parallel and perpendicular bands, Breakdown of Born-Oppenheimer Approximation,

**Raman Spectroscopy:** Polarizability and classical theory of Raman spectrum, Rotational Raman spectra. Vibrational Raman spectra, mutual exclusion principle, Surface enhanced Raman spectra, Resonance Raman,

**Electron Spectroscopy:** Electronic energy states of molecules. Vibrational structure of electronic bands, Electronic transitions and absorption bands, Selection rules, Electron

spectroscopy for chemical analysis (ESCA)-UPS, X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES).

#### Reference Books:

1. I. N. Levine: Quantum Chemistry, Prentice Hall India, 1994.
2. S. N. Datta: Lecture on Chemical bonding and quantum chemistry, 1998.
3. D. A. McQuairrie: Quantum Chemistry, Oxford University press, Oxford, 1982.
4. P. W Atkins: Molecular Quantum Mechanics, Clarendon Press, Oxford, 1983.
5. R. K. Prasad: Quantum Chemistry through Problems and Solutions, New Age International, 1997.
6. F. L. Pilar: Elementary quantum chemistry, Mc-Graw Hill International, 2nd ed. 1990.
7. A. K Chandra: Introduction to Quantum Chemistry, Tata McGraw Hill, 1988. P. W. Atkins, Physical Chemistry, Oxford, London, 6<sup>th</sup> edi, 1998.
8. R. Sindhu, Molecular Spectroscopy, Tata McGraw Hill, 1986.
9. Banwell, Molecular Spectroscopy, Tata McGraw Hill, 1998.
10. I. N. Levine: Quantum Chemistry, Prentice Hall India, 1994.
11. S. N. Datta: Lecture on Chemical bonding and quantum chemistry, 1998.
12. D. A. McQuairrie: Quantum Chemistry, Oxford University press, Oxford, 1982.
13. P. W Atkins: Molecular Quantum Mechanics, Clarendon Press, Oxford, 1983.
14. R. K. Prasad: Quantum Chemistry through Problems and Solutions, New Age International, 1997.
15. F. L. Pilar: Elementary quantum chemistry, Mc-Graw Hill International, 2nd ed. 1990.
16. A. K Chandra: Introduction to Quantum Chemistry, Tata McGraw Hill, 1988. P. W. Atkins, Physical Chemistry, Oxford, London, 6<sup>th</sup> edi, 1998.
17. R. Sindhu, Molecular Spectroscopy, Tata McGraw Hill, 1986.
18. Banwell, Molecular Spectroscopy, Tata McGraw Hill, 1998.
19. Graebeat, Molecular Spectroscopy, Prentice Hall, 1968.
20. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, 1964.

## Semester II

### Physical Methods in Chemistry I

Credits 4

Theory

**Specific objectives:**

To introduce the concepts of different spectroscopic techniques and its application in solving the structures of organic and inorganic compounds.

**Learning outcomes:**

Ensures the students to understand, acquire knowledge on advanced concepts in spectroscopy and thereby structure elucidation of unknown organic and inorganic compounds.

**Electronic Spectroscopic:** Basics of UV Spectroscopy, Applications to Organic Molecules, type of transitions, effect of solvent and substituents, Woodward Fieser rule and applications to polyenes, aromatic compounds and carbonyl compounds

**Infra-Red Spectroscopy:** Principle, instrumentation and sampling techniques, types of stretching and bending vibration – Factors influencing the vibrational frequency, vibrational frequencies of alkane, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenol, carbonyl compounds, amines and heterocyclics– related problems.

**NMR Spectroscopy:**  $^1\text{H}$  NMR, Spectral parameters – intensity, chemical shift, multiplicity, coupling constant, factors affecting chemical shift. Analysis of first order and second - order spectra – shift reagents - structure determination of organic compounds by  $^1\text{H}$  NMR spectra. Chemical shifts and coupling constants (spin-spin coupling) involving different nuclei ( $^1\text{H}$ ,  $^{13}\text{C}$ ) interpretation and applications to inorganic compounds. Examples for different spin systems – chemical shifts and coupling constants (spin-spin coupling) involving different nuclei ( $^1\text{H}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$ ,  $^{13}\text{C}$ ) interpretation and applications to inorganic compounds – Effect of quadrupolar nuclei ( $^2\text{H}$ ,  $^{10}\text{B}$ ,  $^{11}\text{B}$ ) on the  $^1\text{H}$  NMR spectra, Satellite spectra.

Systems with chemical exchange - evaluation of thermodynamic parameters in simple systems – study of fluxional behavior of molecules – an elementary treatment of second order spectra – examples – NMR of paramagnetic molecules – isotropic shifts contact and pseudo-contact interactions – Lanthanide shift reagents

$^{13}\text{C}$  NMR: Proton coupled; off–resonance decoupled; proton noise decoupled  $^{13}\text{C}$  NMR spectra. Assignment of chemical shifts, additivity effect, characteristic chemical shifts of common organic compounds and functional groups, APT, DEPT and INEPT spectra. NMR of common heteroatoms present in organic compounds - 2D NMR techniques  $^1\text{H}$  –  $^1\text{H}$  COSY,  $^1\text{H}$  –  $^{13}\text{C}$  COSY – HMBC, NOESY and INADEQUATE.

**Mass spectrometry:** Elementary idea about mass spectrometry, interpretation of data and solving problems with spectrometric techniques, mass spectra of inorganic and organic molecules

**Microscopic Techniques:** Principles of SEM, AFM, TEM and STM

### Prescribed books

1. Silverstein, R. M., and Webster, F. X., Spectrometric identification of organic compounds, John Wiley and Sons. Inc., 6<sup>th</sup> edition, **1997**.
2. W. Kemp, Organic Spectroscopy, 3<sup>rd</sup> edition, MacMillan, **1994**.
3. Jag Mohan, Organic Spectroscopy: Principles & Applications, Narosa Publishers, **2012**.
4. Drago, R. S., *Physical Methods for Chemistry*, 2<sup>nd</sup> Edition, Saunders College Publishing, **1992**.
5. Lever, A. B. P., *Inorganic Electronic Spectroscopy*, 2<sup>nd</sup> Sub. Edition, Elsevier Science, **1986**.

## Reference Books

1. Pavia, Lampman and Kriz, Introduction to Spectroscopy, Brooks/Cole Pubs Co, 5<sup>th</sup> edition, **2015**.
2. Williams, D. H., and Ian Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill, **1998**.
3. William Kemp, NMR in chemistry: A multinuclear introduction, MacMillan, **1988**.
4. Organic Spectroscopy by L. D. S. Yadav, Kulwer academic publishers, **2004**.
5. Gerson, F., and Huber, W., Electron Spin Resonance Spectroscopy for Organic Radicals, Wiley-VCH, 1st edition, **2001**.
6. Cotton, F. A., and Wilkinson, G., *Advanced Inorganic Chemistry*, 3<sup>rd</sup> edition, Wiley-Eastern Company, New Delhi, **1990**.
7. J. AND Wilkins Lewis, R. G., *Modern Coordination Chemistry Principles and Methods*, Interscience Publishers, Inc., **1967**.
8. Ebsworth, E. A. V., Structural Methods in Inorganic Chemistry, 3<sup>rd</sup> edition, ELBS, Great Britain, **1987**.
9. Scott, R. A., and Lukehart, C. M., Applications of Physical Methods to Inorganic and Bioinorganic Chemistry, John and Wiley & Sons, LTD, **2007**.
10. Solomon, E. I., Lever, A. B. P., Inorganic Electronic Structure and Spectroscopy, Vol., 2, Applications and Case Studies, Wiley-Interscience, **2006**.
11. Satyanarayana, D. N., Electronic Absorption Spectroscopy, Universities Press, **2000**.
12. Jordon, R. B., Reaction Mechanisms of Inorganic and Organometallic Systems, 3rd edition, Oxford University Press, **2007**.
13. Ballhausen, C. J., and Gray, H. B., Molecular Orbital Theory, Benjamin/Cummings Pub. Co, **1965**.
14. Figgis, B. N., and Hitchman, M. A., *Ligand Field Theory and Its Applications*, 1<sup>st</sup> edition, Wiley VCH, **1999**.
15. Huheey, J. E., Keiter, E. A. and Keiter, R. L., and Medhi, O. K., *Inorganic Chemistry - Principles of Structure and Reactivity*, 4<sup>th</sup> Edition, Pearson Education, **2006**.
16. Purcell, K. F. and Kotz, J. C., *Inorganic Chemistry*, Cengage Learning, **2012**.
17. A Carrington and A. D. Mclachlan, Introduction to Magnetic Resonance, Harper & Row, New York, 1979.
18. A. Carrington and Machlachlon, Magnetic Resonance, Harper & Row, 1967.
19. A Derome, Modern NMR Technique, Pergamon, 1983.
20. Farrar and E. D. Becker, Pulsed FT NMR Spectroscopy.
21. Wertz and Bolton, Electron Spin Resonance, McGraw Hill.
22. A. E. Derome, Modern NMR Techniques for Chemistry Research, Pregamon, 1987.
23. C. P. Slichter, Principles of Magnetic Resonance, Third Edition, Springer-Verlag, 1990.
24. T. C. Farrar and E. D. Becker, Pulse and Fourier Transform NMR, Academic Press, New York, 1971.

**Semester II**  
**Advanced Physical Chemistry Laboratory**

**Credit: 4**

**Practical**

**Course objective**

- To know the wet lab chemistry and computational chemistry practical experiments.
- To understand the concept chemical reactions in Kinetics, spectroscopy, surface chemistry, conductometry, potentiometry, viscometry etc.
- To perform Phase diagram with two component and three component systems.
- To know the redox process and determine the cyclic voltammetry method.
- To prove the computational calculate using electrostatic charges, resonance energy, dimerization energy, Gibbs free energy, pKa of the molecules, docking studies etc.

**Course outcome**

After successful completion of this course, the students will able

- To enrich the knowledge about experiments in lab work and in computational work.
- To identify the concentration, adsorption isotherms, surface area, molecular formula, partition coefficient, stability constant, order of rate constant using the chemical compounds.
- To model novel organic/inorganic compounds in their ground state electronic configuration using computational methods.
- To evaluate and study the energy, concentration, structures and kinetics using various spectroscopic methods.

**Part A: List of Wet Lab Chemistry**

(Any 10-12 Experiments)

1. *Surface Chemistry*

- a) Verification of adsorption isotherms (Freundlich and Langmuir): charcoal-acetic acid or charcoal-oxalic acid system.
- b) Kinetics & Determination of surface area by adsorption of acetic acid on Charcoal

2. *Phase Diagram*

- a) Determination of the concentration of the electrolyte using CST of phenol-water system
- b) Three Component Liquid Systems: Acetic Acid – Chloroform – Water

3. *Partition Coefficient*

- a) Partition coefficient of benzoic acid between benzene and water.
- b) Molecular formula of copper-ammonia complex by the partition coefficient method

4. *Spectroscopy*

- a) Formation kinetics of Chromium-EDTA complex (Spectrometry)
- b) Simultaneous Estimation of Manganese and Chromium in a Solution of Dichromate and Permanganate Mixture
- c) Photocalorimetric determination of Bimolecular rate constant

5. *Surface Tension*

- a) Determine the surface excess of amyl alcohol.

6. *Potentiometry*

- a) Titration of a strong and weak Acid Mixture with a Strong Base-Potentiometry  
b) Determination of stability constant of silver diammine complex by potentiometric titrations  
c) Dissociation of a weak acid by potentiometric titration

7. *Conductometry*

- a) Verification of Ostwald's dilution law and determination of dissociation constant of weak acid  
b) Conductometric titrations of a mixture of acids Vs strong base  
c) Van't Hoff's factor of benzoic acid between benzene and water  
d) Critical Micelle concentration of surfactant by conductivity measurements  
e) Verification of Onsager's Equation and Determination of Equivalent Conductance at Infinite Dilution of Strong Electrolytes  
f) Conductometric determination of Nickel using DMG

8. *Kinetics*

- a) Second order rate constant for the alkaline hydrolysis of ethyl acetate by conductivity measurements  
b) Arrhenius parameters for the Acid-Catalysed Hydrolysis of Methyl acetate

9. *Viscometry*

- a) Determination of molecular weight of a polymer by viscosity measurements

10. *Additional*

- a) Specific and molar refraction of a liquid by Refractometry  
b) Reversibility of a redox process and determination of concentration of a given solution by cyclic voltammetry  
c) Inversion of Sucrose-Polarimeter

**Part B: List of Computational Chemistry Experiments**

(Any 3-4 Experiments)

1. Calculation of electrostatic charges of atoms in organic molecules using population analysis
2. Calculation of Resonance energy of aromatic compounds
3. Calculation of dimerization energy of carboxylic acids
4. Perform the conformational analysis of butane using potential energy scan
5. Find the transition state of simple organic reactions and plot the reaction profile.
6. Determination of heat of hydration of organic molecules.
7. Find the Gibbs free energy of simple gaseous phase reactions and calculate equilibrium constant.
8. Calculation of pKa of simple organic molecules and compare it with experimental values
9. Docking studies involving protein ligand interactions.

10. Calculation of electrophilicity index in hard-soft acids and bases.

### Reference Books

1. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn. McGraw Hill, 2009.
3. B. Viswanathan, Practical Physical chemistry, Viva Pub., 2005
4. Saroj Kumar and Naba Kumar, Physical Chemistry Practical, New Central Book Agency, 2012
5. Practical Physical Chemistry Paperback, 1974 by A.M. James, F.E. Prichard.
6. J. Foresman & Aelieen Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 2000.
7. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems, John Wiley & Sons, 2001.
8. D. Rogers Computational Chemistry Using the PC, 3rd Edition, John Wiley & Sons (2003).
9. Leach, Molecular Modelling: Principles and Applications, 2nd Edn, Longman, 2001.
10. J. M. Haile (2001) Molecular Dynamics Simulation: Elementary Methods.

### Semester III Physical methods in Chemistry II

Credit: 4

Theory

#### Specific objectives:

To introduce spectroscopic techniques to solve structure of metal complexes.

#### Learning outcomes:

Ensures the students to understand, acquire knowledge on advanced concepts in spectroscopy thereby able to solve spectrum to structure of metal complexes.

**Electronic Spectroscopy:** Microstates, - terms and energy levels for  $d^1 - d^9$  ions in cubic and square fields – Intensity of bands – group theoretical approach to selection rules - Effect of distortion and spin-orbit coupling on spectra- Orgel and Tanabe-Sugano diagrams – Evaluation of  $10Dq$  and  $\beta$  for octahedral complexes of cobalt and nickel – applications to simple coordination compounds – charge transfer spectra – electronic spectra of  $[\text{Ru}(\text{bipy})_3]^{2+}$ . Electronic Spectra of f-block elements.

Optical rotatory dispersion, circular dichroism and Magnetic circular dichroism – applications to metal complexes. Basic principles of inorganic photochemistry.

**Infrared and Raman Spectroscopy:** Group vibrations and the limitations- combined uses of IR and Raman Spectroscopy in the structural elucidation of simple molecules like  $\text{N}_2\text{O}$ ,  $\text{ClF}_3$ ,  $\text{NO}_3^-$ ,  $\text{ClO}_4^-$  effect of coordination on ligand vibrations – uses of groups vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide – Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal carbonyls with reference to the nature of bonding,

geometry and number of C-O stretching vibrations (group theoretical treatment) – Applications of Raman Spectroscopy – Resonance Raman Spectroscopy.

**EPR spectroscopy:** Theory of EPR spectroscopy - Spin densities and McConnell relationship – Factors affecting the magnitude of g and A tensors in metal species - Zero-field splitting and Kramers degeneracy – Spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes – Applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions. Magnetic properties -Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature independent paramagnetism. Magnetic properties of lanthanides and actinides. Spin crossover in coordination compounds – Single molecule magnets.

**Mössbauer Spectroscopy:** Isomer shifts – Magnetic interactions – Mossbauer emission spectroscopy – applications to iron and tin compounds.

**NQR spectroscopy:** Characteristics of quadrupolar nucleus – effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – applications of NQR spectroscopy.

### Prescribed Books

1. R. S. Drago, *Physical Methods in Inorganic Chemistry*, Van Nostrand Reinhold Inc., U. S., 1965.
2. R. S. Drago, *Physical Methods for Chemistry*, 2nd Edition, Saunders College Publishing, 1992.
3. A. B. P. Lever, *Inorganic Electronic Spectroscopy*, 2nd Sub Edition, Elsevier Science, 1986.
4. J. E. Huheey, E. A. Keiter and R. L. Keiter and O. K. Medhi, *Inorganic Chemistry – Principles of Structure and Reactivity*, 4th Edition, Pearson Education, 2006.
5. A. K. Das and M. Das, *Fundamental concepts of Inorganic Chemistry*, 1<sup>st</sup> Edition, Volume 7, CBS Publishers & Distributors Pvt Ltd. 2014.
6. Wulfborg, G., *Inorganic Chemistry*, University Science Books, 2000.
7. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, Part B: Applications in Coordination, Organometallic, and Bioinorganic Chemistry, Wiley-Interscience; 5<sup>th</sup> edition, 1997.
8. J. Ferraudi, *Elements of Inorganic Photochemistry*, Wiley, New York, 1988.

### Reference Books

1. F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, 3rd ed., Wiley-Eastern Company, New Delhi, 1990.
2. P. J. Wheatley, *The Determination of Molecular Structure*, 2nd Edition, Dover Pubns, 1981.
3. J. AND R. G. Wilkins Lewis, *Modern Coordination Chemistry Principles and Methods*, Interscience Publishers, Inc., 1967.
4. E. A. V. Ebsworth, *Structural Methods in Inorganic Chemistry*, 3rd ed., ELBS, Great Britain, 1987.

5. R. A. Scott and C. M. Lukehart, Applications of Physical Methods to Inorganic and
6. Bioinorganic Chemistry, John and Wiley & Sons, LTD, 2007.
7. E. I. Solomon, A. B. P. Lever, Inorganic Electronic Structure and Spectroscopy, Vol.,2 Applications and Case Studies, Wiley-Interscience, 2006.
8. B. P. Lever, Inorganic Electronic Spectroscopy, 2nd Sub Edition, Elsevier Science, 1986.
9. D.N. Satyanarayana, Electronic Absorption Spectroscopy, Universities Press, 2000.
10. R.B. Jordon, Reaction Mechanisms of Inorganic and Organometallic Systems, 3<sup>rd</sup> Edition, Oxford University Press, 2007.
11. C.J. Ballhausen and H.B. Gray, Molecular Orbital Theory, Benjamin/Cummings Pub. Co, 1965.
12. N. Figgis and M. A. Hitchman, *Ligand Field Theory and Its Applications*, 1<sup>st</sup> Edition, Wiley VCH, 1999.
13. A.W. Adamson, Inorganic Photochemistry, John Wiley & Sons, New York.
14. S.F.A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach,
15. Spectrum Academic Publishers, Oxford University Press, 1996.
16. W. Adamson and P. D. Fleischauer, Concepts of Inorganic Photochemistry, Wiley, New York, 1975.

### Semester III

#### Reagents & Synthetic Strategies in Organic Chemistry

**Credit: 4**

**Theory**

**Specific objectives:**

To introduce the advanced synthetic methodologies involving modern synthetic reagents, protecting groups and planning organic synthesis.

**Learning outcomes:**

Ensures the students to understand, acquire knowledge on modern synthetic reagents, protecting groups and planning of organic synthesis through disconnection approach.

**Protecting and Deprotecting Strategies:** Need for protection and deprotection of functional groups during chemical reactions- protection of hydroxyl, mercapto, amino, carbonyl and carboxylic groups.

**Planning Organic Synthesis:** An introduction to retrosynthesis - Synthons – synthetic equivalent – target molecule, functional group interconversion. Disconnection approach- one group disconnection- disconnection of alcohols, olefins and ketones. Logical and illogical disconnections. Two group disconnection-1,2, -1,3, 1,4, 1,5 and -1,6 dioxygenated skeletons and dicarbonyls; Umpolung, antithesis, chiron. C-C bond forming reactions (alkylation as well as enamine alkylation). Retro Diels – Alder reactions- Pericyclic reactions- Retrosynthesis of heterocycles containing two nitrogens. Designing synthesis: Disconnection approach in Camphor, reserpine and longifolence,

**Synthetic Reagents:** Use of the following reagents in organic synthesis and functional group transformations: Sodium borohydride, tri-n-butyl tin hydride, lithium dimethyl cuprate,

lithium diisopropyl amide, trimethyl silyl iodide, diborane, ozone, CrO<sub>3</sub> DCC, DDQ, 9-BBN, lead tetra acetate, phenyl iodoso acetate, dimethyl sulphoxide, SeO<sub>2</sub>, PCC, Yeast. Phase transfer catalysis – benzyltriethylammonium halides- crown ethers.

Functional group transformations using reducing reagents: Use of NaBH<sub>4</sub>, NaCNBH<sub>3</sub>, LiAlH<sub>4</sub> and Bu<sub>3</sub>SnH; Use of Sn/HCl, Zn/HCl, Hydrazine, Li-NH<sub>3</sub>, Na/alcohol, Pd/H<sub>2</sub> and Raney Ni.

### Prescribed books

1. Smith M. B., March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th edn, Wiley, **2015**
2. Carey, F.A., Sundberg, R.J., Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edn, Springer, **2007**.
3. Carey, F.A., Sundberg, R.J., Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th edn, Springer, **2007**.
4. Clayden, J., Greeves, N., Warren, S. Organic Chemistry, 2nd edn, Oxford University Press, **2014**
5. Li, J. J., Corey, E. J., Name Reactions for Homologation, Part 1, Wiley-Blackwell, **2009**
6. Mundy, B. P., Ellerd, M G., Favalaro Jr. F. G., Name Reactions and Reagents in Organic Synthesis, 2nd edn, Wiley-Blackwell, **2005**
7. Carruthers, W., Coldham, I., Modern Methods of Organic Synthesis, 4th edn, Cambridge University Press, **2015**
8. Norman, R. O. C., Coxon, J. M., Principles of Organic Synthesis, 3rd edn, **1993**.
9. Wyatt, P., Warren, S., Organic Synthesis: Strategy and Control, Wiley-Blackwell, **2007**
10. Warren, S., Wyatt, P., Organic Synthesis: The Disconnection Approach, Wiley, **2008**
11. Corey, E. J., Cheng, X. M. The Logic of Chemical Synthesis, Wiley-India Private Ltd, **2011**
12. Nicolaou, K. C., Sorensen, E. J., Classics in Total Synthesis, Wiley-ECH, **1996**

**Semester III**  
**Thermodynamics (Classical & Statistical) and Electrochemistry**

**Credit: 4**

**Theory**

**Course objective:**

- To know the concepts of classical as well as statistical Thermodynamics
- To study about the Basic and essential of electrochemistry in distinct phenomena (in Equilibrium and Dynamic).
- To understand the tuned concept of electrochemistry in storage cells.
- To aware about the recent applications using the concepts of electroanalytical techniques.

**Course outcome:**

After successful completion of this course, the students will able

- To enrich the knowledge about the basic laws of thermodynamics and fundamentals of statistical thermodynamics.
- To observe the electrochemical ideas at equilibrium and dynamics progress.
- To familiar in storage cells concepts using the principle of electrochemistry.

**Classical Thermodynamics**

**Introduction:** Laws of thermodynamics, Entropy- Free Energy-Systems of Variable Compositions - Fugacity and Activity Maxwell's relations – significance, Partial molar properties – Chemical potential, Fugacity and Activity. Concept of absolute entropy and residual entropy

**Thermodynamics of mixing:** Thermodynamic functions of mixing, Clausius Inequality, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law, excess thermodynamic functions

**Chemical Equilibrium:** Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- van't Hoff equations.

**Third law of thermodynamics:** Nernst heat theorem, development of third law of thermodynamics, determination of absolute entropies using third law, entropy changes in chemical reactions.

**Thermodynamics of Irreversible Processes:** Thermodynamics of irreversible processes with simple examples. phenomenological relations. Onsager reciprocal relations - principle of microscopic reversibility. Electrokinetic phenomena. Thermoelectric phenomena.

**Statistical Thermodynamics**

**Fundamentals of Statistical Thermodynamics:** Thermodynamic probability, Stirlings approximation microstate and macrostate, entropy and probability, most probable distribution, Maxwell - Boltzman statistics. Distribution Law-Effect of temperature on distribution, Calculation of most probable velocity, average and mean square velocity, components of velocity, Mean free path, Effusion and diffusion, thermal conductivity and viscosity of gases. Heat capacity of gases - classical and quantum theories, heat capacity of hydrogen

**Partition and Thermodynamic Functions:** Partition function and its relation to thermodynamic properties, Translational, rotational and Vibrational partition function. Heat

capacity of solids: Dulong - Petits law, Einstein's theory and its modification, Debye's theory of heat capacity of solids.

**Quantum statistics:** Bose - Einstein statistics & distribution, example of particles, Bose-Einstein condensation, difference between first order and higher order phase transitions, liquid helium, supercooled liquids. Fermi - Dirac statistics, Fermi-Dirac distribution: examples of particles, application in electron gas, thermionic emission. Comparison of three statistics

### **Electrochemistry**

Activity and Activity coefficient of electrolytes, ionic strength, Debye Huckel theory of strong electrolytes, Debye Huckel limiting law, Mean ionic activity coefficient. Application of Debye Huckel theory to - Relaxation and electrophoretic effects, Debye-Huckel-Onsager equation and its derivation. Debye Falkenhagen effect. Wien effect. Ionic activity coefficients of strong electrolytes- Derivation of Debye-Huckel limiting law.

**Equilibrium Electrochemistry:** EMF Phenomena, Cell Potential and its measurement, reference electrodes. Electrochemical cells, concentration cells and activity coefficient determination, liquid junction potential, Determination of solubility. pH Conductometric, Potentiometric and pH titrations, Redox indicators and redox titrations.

**Dynamic Electrochemistry:** Electrical double layer, various models of electrical double layer, Electrode polarization. Overpotential, hydrogen and oxygen overvoltage, theories of overvoltage, Butler-Volmer equation for simple electron transfer reactions, Tafel plot and its significance, Corrosion: stability of metals, Pourbaix diagram-Evan diagram-corrosion control and methods for prevention.

**Storage cells:** Lead acid battery, Lithium battery, nickel cadmium cell. Fuel Cell. Theory and working of fuel cell. H<sub>2</sub>- O<sub>2</sub> fuel cell, methanol fuel cell, Solid oxide fuel cells.

**Electroanalytical Techniques:** Polarography – diffusion current, supporting electrolyte, three electrode system, polarographic maxima. Amperometry – principles and applications – Types of amperometry. Cyclic voltammetry – principles, applications. Stripping voltammetry.

### **Reference Books**

1. R.P. Rastogi, R.R. Mishra, An introduction to Chemical Thermodynamics, Vikas publishing house, **2009**.
2. J. Rajaram, J.C. Kuriakose, Thermodynamics, S Chand and Co., **1999**.
3. M.C. Gupta, Statistical Thermodynamics, New age international, **2007**.
4. L.K. Nash, Elements of Classical and Statistical Mechanics, 2<sup>nd</sup> Edn. Addison Wesley, **1972**.
5. F.W. Sears, G.L. Salinger, Thermodynamics, Kinetic Theory and Statistical Thermodynamics, Addison Wesley, **1975**.
6. J. Kestin, J.R. Dorfman, A Course in Statistical Thermodynamics, Academic Press, **1971**
7. John E. Freund. Modern elementary statistics, **2003**, ISBN-13: 978-0131874398 20.
8. S. P. Gupta, Statistical Methods: S. Chand, **2014**.
9. J. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2B, 2<sup>nd</sup> Edn., Wiley, New York, **1998**
10. D.R. Crow, Principles and Applications of Electrochemistry, Chapman & Hall, 3<sup>rd</sup> Edn., New York, **1994**

11. S. Glasstone, Introduction to Electrochemistry, Biblio Bazar, **2011**.
12. B.K. Sharma, Electrochemistry, Krishna Prakashan, **1985**.
13. A.I. Vogel, A Textbook of Quantitative Analysis including Instrumental Analysis, John Wiley & Sons, **1961**.
14. H.H. Willard, J. A. Dean, L.L. Merritt, Instrumental Methods of Analysis, Van Nostrand, **1965**.
15. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn. Saunders College Pub., **2007**.

### Semester III

#### Advanced Inorganic Chemistry Laboratory

**Credit: 4**

**Practical**

**Specific objectives:**

To introduce multistep inorganic compound synthesis and purification, separation and spectroscopic analysis. Estimation of metal ions by spectrophotometry.

**Learning outcomes:**

Ensures the students to understand, acquire knowledge and have hands on experience in multistep inorganic compound synthesis and analysis by using spectroscopic techniques, Separation techniques.

Preparation of the following compounds and their Characterization

1. Tetramminecopper(II) sulphate.
2. Potassium trioxalatochromate(III).
3. Potassium trioxalatoaluminate(III).
4. Trithiourea copper(I) chloride.
5. Dibenzyltin dichloride.
6. Nitro and nitrito linkage isomers
7. Mn<sub>3</sub> clusters

1. Synthesis and study of Tris(oxalato)iron(III) potassium salt by Cyclic Voltammetry (CV) and Differential Pulse Voltammetry (DPV), and determination of the following: the formal reduction potential ( $E_0'$ ); the number of electrons transferred in the redox process (n); electrochemical reversibility.
2. Synthesis and study of Mn<sup>III</sup>(Salen)Cl by Cyclic Voltammetry and Differential Pulse Voltammetry (DPV), and determination of the following: the formal reduction potential ( $E_0'$ ); the number of electrons transferred in the redox process (n); electrochemical reversibility.
4. Preparation and determination of the effective magnetic moment and number of unpaired electrons in Mn(acac)<sub>3</sub>.
5. Preparation and determination of the aquation rate of [Co(NH<sub>3</sub>)<sub>5</sub>Cl]Cl<sub>2</sub>.
6. Preparation and resolution of the optically active compound [Co(en)<sub>3</sub>]<sup>3+</sup>.
7. Preparation and characterization of (Mesitylene)tricarbonylmolybdenum(0) by solution infrared spectrum.
8. Bioanalytical techniques – Monitoring the cleavage of DNA and protein by metal complexes using Gel electrophoresis techniques – Agarose and PAGE (Demo only).

## Reference Books

1. Elias, A. J., A Collection of Interesting General Chemistry Experiments, Universities Press, Sangam Books Ltd, **2002**.
2. Woollins, J. D., Inorganic experiments, 3rd edition, Wiley-VCH Verlag GmbH @ Co. KGaA, **2012**.
3. Hein, M., Peisen, J. N., and Miner, R. L., Foundations of College Chemistry in the Laboratory, John Wiley and Sons, **2011**.
4. Girolami, G. S., Rauchfuss, T. B., and Angelici, R. J., Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, 3rd edition, University Science Books, **1999**.
5. Jolly, W. L., The Synthesis and Characterization of Inorganic Compounds, Prentice-Hall, Inc. **1970**.
6. In-house Laboratory Manual, Department of Chemistry, CUTN.
7. Ghoshal, Mahapatra and Nad, An Advanced Course in Practical Chemistry, New Central Book Agency, **2011**.

## Semester IV Project

Credit: 12

Practical

## List of Electives

Course Code	Title of the Course	Credits
CHEE01	Principles of Polymer Science	4
CHEE02	Principles of Fluorescence Spectroscopy	4
CHEE03	Asymmetric Catalysis	4
CHEE04	Essentials of Carbohydrate Chemistry	4
CHEE05	Organic Electronics	4
CHEE06	Photochemistry in Molecules and Materials	4
CHEE07	Medicinal Inorganic Chemistry	4
CHEE08	Organic Semiconductors	4
CHEE09	Advances in Polymer Science	4
CHEE10	Advances in Carbohydrate Research	4
CHEE11	Advanced Organic Materials and Catalysis	4
CHEE12	Chemistry of CH Activation	4
CHEE13	Advanced Bio-inorganic Chemistry	4
CHEE14	Principles of Biochemistry	4
CHEE15	Mathematics for Chemists and biologists	4
CHEE16	Electrochemical Energy Systems	4
CHEE17	Fundamentals of Analytical Chemistry	4
CHEE18	Computational Chemistry	4
CHEE19	Supramolecular Chemistry	4
CHEE20	Mathematical methods in Chemistry	4
CHEE21	Organometallics, Catalysis and Inorganic Spectroscopy	4
CHEE22	Physical methods in Chemistry	4

CHEE23	Applications of Computational Methods in Chemistry	4
CHEE24	Chemical Lab Safety and Management	4
CHEE25	Advances in Organic Chemistry	4
CHEE26	Green Chemistry	4
CHEE27	Selected topics in synthetic organic Methods	4
CHEE28	Advanced Topics in Organometallic Chemistry	4
CHEE29	Industrial Chemistry	3
CHEE30	Advanced Organic Nanomaterials	4
CHEE31	Computer software for Chemists (SEC)	2
CHEE32	Water and wastewater analysis (SEC)	2

\* New electives will be appended based on the availability of course instructor.  
 Electives will be offered based on the individual faculties' availability