# Semester-IV

**Fourth Semester**
**Core Course**
**Course Title: Advanced Inorganic Chemistry**
**Course Code: CHM651C**

Credits = 4
M.M. = 100
L T P=3 1 0

**Course Learning Outcomes:** After completion of this course, the students will be able to

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|---|---|
| **CLO 1:** | Understand the application of symmetry with respect to vibrational and Raman spectroscopy |
| **CLO 2:** | Know about the application of symmetry with respect to MOT, VBT and Electronic transition |
| **CLO 3:** | Learn about photophysical properties and photochemical reactions in transition metal complexes |
| **CLO 4:** | Learn about synthesis, characterization and applications of porous materials containing metal ions and organic linkers. |

**Unit I: Symmetry Aspects of Molecular Vibrations** **(Contact hours: 16)**

Construction of character tables for $C_4v$, $D_{3h}$, $D_3d$ and $T_d$. Application of group theory to IR and Raman spectroscopy, Symmetry of IR and Raman active normal vibrational modes of $AB_2$, $AB_3$, $AB_4$, $AB_5$ and $AB_6$ type molecules. Contribution of internal coordinates to normal modes for $H_2O$ molecule, Symmetry selection rules for fundamental vibrational transitions (qualitative treatment).

**Unit II: Symmetry Aspects of Hybrid and Molecular Orbitals** **(Contact hours: 16)**

Transformation properties of atomic orbitals, Hybrid orbitals for sigma bonds in trigonal planar ($BCl_3$), Tetrahedral ($CH_4$), Square planar $[PtCl_4]^{2-}$, trigonal bipyramidal ($PF_5$), square pyramidal ($ML_5$) and octahedral geometry ($ML_6$), Hybridization scheme for pi bonding in Square Planar and tetrahedral systems, Molecular orbitals for sigma bonding in trigonal planar and tetrahedral systems, Applications of symmetry to Molecular chirality, Polarity and Fluxionality

**Unit III: Inorganic Photochemistry** **(Contact hours: 16)**

Excited states in transition metal complexes: Ligand field Intra-ligand and charge transfer excited states and metal centered excited states. Photo-physical properties: rate constants and quantum yields, Potential energy surfaces of states and Jablonoski diagrams

Photochemical reactions: Substitution and redox reactions of Cr(III), Co(III), Rh(III) and Ru(II) complexes, manganese-based photosystems for the conversion of water into oxygen, Metal complex sensitizers, electron relay, semiconductor supported metal oxide systems, water photolysis, nitrogen fixation and $CO_2$ reduction

**Unit IV: Metal Organic Frameworks** **(Contact hours: 16)**

Introduction, porous coordination polymers, frameworks with high surface area, Lewis acid frameworks, soft porous crystals, design of metal organic frameworks and design of functional metal organic frameworks by post-synthetic modification. Lanthanide based MOFs, Applications of metal organic frameworks-separation and purification of gases by MOFs, hydrogen storage, MOFs in the pharmaceutical world.

**Books Recommended:**


1. Chemical Applications of Group Theory, F. A. Cotton, Wiley NY, 3rd Edn.; 1990
2. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, 2nd Edn.; 2009
3. Photochemistry, Carol J. Wayne and Richard P. Wayne; Oxford University Press; 1996.
4. Metal-Organic Frameworks: Applications from Catalysis to Gas Storage, David Farrusseng, Wiley-VCH, Year: 2011.


**Reference Books:**


5. Group Theory and Symmetry in Chemistry; Lowell H. Hall.; McGraw-Hill, 1969
6. Fundamentals of Photochemistry; C Rohatgi, Mukhergi; Wiley Eastern.; 1992
7. Introduction to Reticular Chemistry: Metal-Organic Frameworks and Covalent Organic Frameworks, Omar M Yaghi; Markus J Kalmutzki; Christian S Diercks, Wiley-Vch, Year: 2019.
8. Introduction to zeolite science and practice, H. Van Bekkum, E. M. Flanigen, P. A. Jacobs, J. C. Jansen, Elseviver Pub. Amsterdam, 2001
9. Zeolite molecular sieves: structure, chemistry, and use, Donald W. Breck, John Wiley & Sons N.Y. (1974).
10. Applications of Inorganic Photochemistry; J. Chem. Edu.; Vol.74, No 69. 1997

**Fourth Semester**
**Core Course**
**Course Title: Advanced Organic Chemistry**
**Course Code: CHM652C**

Credits = 4
M.M. = 100
L T P=3 1 0

**Course Learning Outcomes:** After completion of this course, the students will be able to:

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|---|---|
| **CLO 1:** | Acquire the knowledge of designing of organic syntheses using retrosynthetic analysis of organic compounds (disconnection approach). |
| **CLO 2:** | Understand the importance, classification, structural determinations, and synthesis of natural products |
| **CLO 3:** | Learn classification of drugs, lead compounds and their modifications, SAR analysis and prodrugs and their applications in medicinal chemistry |
| **CLO 4:** | Learn nomenclature, structure and reactivity, synthesis and applications of heterocyclic compounds |

**Unit I: Retrosynthetic Analysis** (Contact hours: 14)

An introduction to synthons and synthetic equivalents, The importance of order of events in organic synthesis, Functional group interconversion, The disconnection approach. One group, two group and electrocyclic disconnections, Examples involving connections and rearrangements.
Protection of functional groups: Principle of protection of carbon-hydrogen bonds (in terminal alkynes and hydrogens of aldehydes), Carbon-carbon double bonds, Alcoholic hydroxyl groups, Amine groups, Carbonyl and carboxyl groups.

**Unit II: Natural Products** (Contact hours: 16)

Introduction to natural products, classification, and their importance in drug discovery.
**Terpenoids:** Isoprene rule, Classification, Nomenclature, General methods of structure determination, Stereochemistry and synthesis of α-Pinene, Menthol, Farnesol. Biosynthetic routes to mono and sesquiterpenoids. Essential oils, their chemical composition, Extraction, Methods of analysis.
**Alkaloids and flavonoids:** Introduction, classification, nomenclature and general methods of structure determination, biosynthesis of flavonoids. Medicinal applications of flavonoids and alkaloids.

**Unit III: Medicinal Chemistry** (Contact hours: 16)

Classification and sources of drugs, concept of lead compounds and lead modification, Analogues, Structure activity relationship (SAR): isosterism, bioisosterism, changing the size and shape, number of methylene groups in chain, degree of unsaturation, Effect of introduction of methyl groups, Halogens, Hydroxyl, Carbonyl, thiols sulphides groups and introduction/removal of ring systems on pharmacological activity. Prodrugs and types of prodrugs.

**Unit IV: Heterocyclic Chemistry** (Contact hours: 16)

Nomenclature of heterocycles (Hantzsch-Widman nomenclature, Replacement nomenclature), non-aromatic and aromatic heterocycles. Structure of five membered, six membered and bicyclic heteroatomic systems, Aromaticity of various heterocyclic systems, Resonance energies. Mesoionic systems. UV/Visible and NMR spectroscopy of heterocycles. Reactivity of aromatic heterocycles. Synthesis of aromatic heterocycles, Reaction types most frequently used in heterocyclic ring synthesis, Cyclisation, Cycloaddition, Electrocyclic processes in heterocyclic ring synthesis.

**Books Recommended:**


1. Heterocyclic Chemistry, J. A. Joule and K. Mills 4th Edn., (Black Well Science. 2000).
2. Medicinal Chemistry- An Introduction, Gareth Thomas (Wiley-2000). 3rd Edn;.
3. Medicinal Chemistry, Ashutosh Kar. (Wiley Eastern-1993).
4. Designing Organic Synthesis, S. Warren (Wiley-1978).


**Reference Books:**


5. Organic Synthesis- concept, methods and Starting Materials, J. Furhop and G. Penzlin (Verlag VCH-1986).
6. Some Modern Methods of Organic Synthesis, W. Carruthers 3rd Edn., (Cambridge University Press-1986).
7. Modern Synthesis Reactions, H.O. House 2nd Edn. (W. A. Benjamin, NY-1972).
8. Principles of Organic Synthesis, R. O. C. Norman (Chapman and Hall-1978).
9. Heterocyclic Chemistry, Thomas. L. Gilchrist, Prentice Hall; 3rd Edn; April 14, 1997.
10. Introduction to strategies for organic synthesis, Laurie S. Starkey, First Edition, John Wiley & Sons, 2018.

**Forth Semester**
**Core Course**
**Course Title: Advanced Physical Chemistry**
**Course code: CHM653C**

Credits = 4
M.M. = 100
L T P=3 1 0

**Course Learning Outcomes:** After completion of this course, the students will be able to:

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| **CLO 1:** | Understand the stability of conjugated linear and cyclic polyenes in light of Huckel MO theory and Hartree-Fock approximations for multi-electron system. |
| **CLO 2:** | Understand the relationship between microscopic features of component molecules and macroscopic aspects of a system |
| **CLO 3:** | Use equilibrium statistical mechanics tools and methodologies to investigate and evaluate various aspects of chemical systems |
| **CLO 4:** | Acquire the knowledge of the practical application of micellar's systems in solubilization of poorly soluble biomolecules and drugs, catalysis. and drug delivery. Further acquaint them with various theoretical and mathematical models used in surface chemistry. |

**Unit I: Quantum Chemistry-IV** **(Contact hours: 16)**

Huckel's Pi-MO theory, Application to linear and cyclic polyenes, Aromaticity, Pi-electron charge and pi-bond-order. Alternant hydrocarbons, Naphthalene. Limitations of Huckel theory.

Self-Consistent field method: Hamiltonian and wave function for multi-electron systems, Molecular and Electronic Hamiltonians, Hartree products and their limitations, Antisymmetrized wave function, Slater-determinant, Hartree-Fock self-consistent field method in the light of minimal basis $H_2$ molecule system; one and two electron integrals. General polyelectronic system, Coulomb and exchange operators and integrals. Basic procedure of a self-consistent field method.

**Unit II: Statistical Thermodynamics-I** **(Contact hours: 16)**

Concept of Distribution, thermodynamic probability and most probable distribution, Sterling approximation, Derivation of Boltzmann distribution law, Bose-Einstein, and Fermi-Dirac distribution equations (without derivation). Comparison of M-B, F-D and B-E distribution laws, Partition function and its significance, translational, rotational, vibrational, and electronic partition function, Calculation of thermodynamic properties in terms of partition functions, application to ideal monoatomic gas, Equilibrium constant in terms of Partition Functions, Application to dissociation equilibrium.

**Unit III: Statistical Thermodynamics-II** **(Contact hours: 16)**

Thermodynamic properties of a diatomic gas. Calculation of equilibrium constant using partition functions; examples of isotope exchange reaction, $H_2 + O_2$ reaction, reaction between $C_2H_4$ and $H_2$.

Concept of ensembles, ensemble average and postulate of equal a priori probability. Canonical, Grand-canonical and Micro-canonical ensembles. Perfect gas in canonical ensemble, Entropy and free energy. Grand partition function and its characteristic equation. Ideal-Fermi Dirac gas: electrons in metals, Black body radiation, Bose-Einstein condensation.

Einstein model of energy and heat capacity of a solid using canonical partition function. Limitations of Einstein model, Debye model of heat capacity.

**Unit IV: Micelles, Solubilization and Micellar Catalysis** **(Contact hours: 16)**

Surfactants: Classification, Kraft temperature and cloud point. Micellization: Critical micelle concentration (cmc), Aggregation number (N), Counterion binding. Factors affecting cmc and N in aqueous media, Structure and shape of micelles: Chain packing, Variation of micellar size and shape with surfactant concentration and organic additives. Thermodynamics of micellization: Pseudophase and mass action models.

Mixed Micelle formation (two components): Clint equation, Rubing equation.

Solubilization and factors affecting solubilization, Nature of surfactant/solubilizate, Additive and temperature, Solubilization of drugs into micelles and its importance in drug delivery systems and controlled release.

Micelles as reaction media: Theoretical consideration of reactions in micellar media, Examples of micellar catalysis for hydrolysis, Oxidation and reduction reactions.

**Books Recommended:**


1. Modern Quantum Chemistry Introduction to Advanced electronic structure theory. A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
2. Quantum Chemistry- Ira. N. Levine, Prentice Hall, 7th Edn.; 2013.
3. Statistical Thermodynamics, M. C. Gupta, New Age Publishers Pvt Ltd., 2013
4. Statistical Mechanic by D. A. McQuarie, Viva Books Pvt Ltd, 2018.


**Reference Books:**


5. Statistical Thermodynamics by T. Hill, Dover publications, 2012.
6. Introduction of Statistical Thermodynamics, R.P.H. Gasser and W.G. Richards, World Scientific, Singapore (1995).
7. Foundations of Colloid Science, Robert J. Hunter, Oxford University Press, New York, 2007.
8. Principles of Colloid and Surface Chemistry, P.C. Heimenz, Marcel Dekker Inc. New York, 1986.
9. Surfactants and Interfacial Phenomena, M. J. Rosen, John Wiley & Sons, New York, 2004.
10. Surfaces, Interfaces and Colloids, D. Y. Meyer, VCH Publishers, Inc. 1991.

**Fourth Semester**
**Core Course**
**Course Title: Nanotechnology and Nanoscience**
**Course code: CHM654C**

Credits = 4
M.M. = 100
L T P=3 1 0

**Prerequisites:**

**Course Learning Outcomes:** After completion of this course, the students will be able to….

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| **CLO 1:** | To provide information about classification of nanomaterials along with optical, electric and magnetic properties |
| **CLO 2:** | To illustrate about different approaches for synthesis of nanomaterials |
| **CLO 3:** | To provide detailed introduction about polymer reactions and control and understating of structure of polymers |
| **CLO 4:** | To understand how we can tune polymers structure after learning characterization techniques |

**Unit I: Nanoscience and Nanomaterials** **(Contact hours: 16)**

Nanoscience and nanotechnology, Nanostructures in nature, Classifications of nanomaterials-zero dimensional-one dimensional-two dimensional-three dimensional nanostructures, Quantum structures-Quantum dots-Quantum wire Quantum well, Surface effects of nanomaterials, Surface plasmon resonance, Quantum size effects, Effect of size on properties: reactivity, optical, electrical, and magnetic properties.

Carbon Nanotubes, single walled carbon nanotubes (SWCNT's), multiwalled carbon nanotubes (MWCNT's), Metalic nanomaterials (Au, Ag, Pd, Cu) - Metal oxide nanomaterials (TiO2, CeO2, ZnO, MgO), Semiconductor nanomaterials (Si, Ge, CdS, ZnSe) and ceramics.

**Unit II: Synthesis of Nanomaterials** (Contact hours: 16)

Nano-materials synthesis, Top-down and bottom-up approaches, Mechanical attrition (Ball Milling and Tube milling), Lithography, Co-precipitation, Sol-Gel Method. Solvothermal synthesis, Hydrothermal synthesis, Chemical Vapor deposition, Plasma Synthesis method, sonochemical Process, Reverse micellar/Micro-emulsion method, Reverse micelles as nano reactors. Introduction to characterization of Nanomaterials.

**Unit III Polymerization Reactions and Kinetics**

Introduction and importance of polymers; Basic concepts: monomers, repeat units, degree of polymerization; Classification of polymers: skeletal structures, monomer arrangements, properties and polymerization mechanism; Polymerization reactions: linear step polymerization, Carothers theory, statistical theory, non- linear step polymerization, Chain polymerization- free radical, cationic, anionic and coordination; Kinetics of chain polymerization.

**Unit: IV Polymer Characterization**

Polydispersion and average molecular weight concept: Number, weight & viscosity average molecular weights; Measurement of molecular weights: End-group, membrane osmometry, light scattering and viscometry; Polymer crystallization, morphology and chain tacticity; Melting (Tm) and glass transition(Tg) temperature, effects of molecular weight, diluents, chemical structure, branching and cross linking, relationship between Tm and Tg; Thermal analysis and visco-elastic properties.

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**Books Recommended:**


1. Nanochemistry: A Chemical Approach to Nanomaterials, Geoffrey A. Ozin, André C. Arsenault, Ludovico Cademartiri, 2nd Edn: 2008
2. Optical properties and spectroscopy of nanomaterials: Jin Zhong Zhang, World scientific, 2009.
3. Textbook of Polymer Science, F.W. Billmeyer Jr., John Wiley & Sons, Inc., 2000.
4. Introduction to Polymers, R.J. Young and P.A. Lovel, Chapman & Hall, London.


**Reference Books:**


5. Physical Principles of Electron Microscopy: An introduction to TEM, SEM and AFM by R. F. Eqerton, Springer, 2nd Edn: 2016.
6. Nano Materials, B. Viswanathan, Narosa Publications, 2014.
7. Nanotechnology, J. Ramsden, Elsevier, 1st Edn.: 2011.
8. Principles of Polymerization, G. Odian, John Wiley & Sons, Inc., New York.
9. Polymer Science and Technology, Joel Fried, Prentice Hall PTR, ISBN : 0130181684
10. Polymer Chemistry: An Introduction, Malcolm P. Stevens, Oxford University Press

**Fourth Semester**
**Core Course**
**Course Title: Project and Dissertation**
**Course Code: CHM655C**

Credits = 4
M.M. = 100
L T P=0 0 4

**Prerequisites:**

**Course Learning Outcomes:** After completion of this course, the students will be able to:

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| **CLO 1:** | Design and develop research skills |
| **CLO 2:** | Learn about how to write review of literature |
| **CLO 3:** | Obtain hands-on experience on various instruments and theoretical tools |
| **CLO 4:** | Find solution for social problems with relevance to environment, health, materials, water treatment and drug development |

- In this course, the student will choose a lab-oriented problem and perform theoretical and practical work after reviewing literature from different sources.
- The student will be guided by a faculty during this course and will have to submit a short synopsis, duly verified by the faculty, project coordinator and Head of the Department.
- The student will have to submit a dissertation based on the problem chosen by him/her (after consultation with the guide) during this course to the Department for evaluation.
- The student will also have to give a seminar about the literature surveyed and work done during this course.