M.Sc.

School of Chemistry

(Based on UGC – Learning Outcomes-Based Curriculum Framework)

Vision Statement:

To be the source of knowledge and center of training that imparts a sound foundation in chemical sciences with strong transdisciplinary reach, and spawns original and innovative research in contemporary and futuristic chemical themes.

Mission Statements:

- Providing quality chemical sciences education at masters and doctoral levels
- Conducting fundamental and advanced research in chemical sciences
- Establishing research collaborations with other universities/institutes/laboratories
- Carrying out sponsored research and development projects from international/national government and private partners

Qualification Descriptors (QDs)

Utilizing basic knowledge and laboratory skills gained in chemical sciences to:

QD-1 analyze, interpret and explain chemically relevant observations

QD-2 identify critical scientific issues and provide potential resolutions

QD-3 create/cultivate new generations of human resource in chemical sciences

QD-4 formulate innovative and relevant chemical problems and develop solutions

Mapping Qualification Descriptors (QDs) with Mission Statements (MS)

	MS-1	MS-2	MS-3	MS-4
QD-1	3	3	1	1
QD-2	3	3	1	1
QD-3	3	3	2	1
QD-4	3	3	3	3

Program Learning Outcomes (PLOs)

After going through the two years of study, chemistry graduates can use the comprehensive knowledge and skills gained, to:

PLO-1: observe, analyze and interpret chemical phenomena and process

PLO-2: design and develop new molecules/processes with industrial and societal applications

PLO-3: formulate new ideas/concepts in chemical sciences and test them

PLO-4: communicate effectively the principles and practice of chemical sciences

PLO-5: address issues of environment, health and development from a chemical perspective

PLO-6: follow professional ethics in all spheres of activity

PLO-7: function effectively as a member/leader in diverse teams/groups

PLO-8: engage in independent learning in the broadest context of scientific advancement

Mapping of Program Learning Outcomes (PLOs) with Qualification Descriptors (QDs)

	QD-1	QD-2	QD-3	QD-4
PLO-1	**3**	**3**	**2**	**2**
PLO-2	**3**	**3**	**2**	**3**
PLO-3	**3**	**3**	**2**	**3**
PLO-4	**2**	**2**	**3**	**2**
PLO-5	**2**	**2**	**3**	**3**
PLO-6	**1**	**1**	**3**	**2**
PLO-7	**3**	**3**	**3**	**3**
PLO-8	**3**	**3**	**3**	**3**

Course Structure

I Year					
I Semester (*20 credits*)			**II Semester (*24 credits*)**		
Number	**Title**	**Credit**	**Number**	**Title**	**Credit**
CY-401	Basic concepts and coordination chemistry	3	CY-451	Main group and inner transition elements	3
CY-402	Physical organic chemistry	3	CY-452	Organic reactions and mechanisms	3
CY-403	Quantum chemistry	3	CY-453	Molecular spectroscopy	3
CY-404	Inorganic chemistry lab: Quantitative and qualitative analysis	3	CY-454	Chemical and statistical thermodynamics	3
CY-405	Organic chemistry lab: Techniques	3	CY-455	Biological chemistry	3
CY-406	Computer programming laboratory	2	CY-456	Inorganic chemistry lab: Synthesis	3
FN-106	Symmetry and Mathematics	3	CY-457	Physical chemistry lab	3
				[Any Foundation Course]	3
II Year					
III Semester (*21 credits*)			**IV Semester (*15 credits*)**		
Number	**Title**	**Credit**	**Number**	**Title**	**Credit**
CY-501	Spectroscopic methods for structure elucidation	3	CY-551	Chemistry of materials	3
CY-502	Advanced organic synthesis	3	CY-552	Seminar	3
CY-503	Chemical dynamics	3	CY-553	Project	3
CY-504	Chemical binding	3			
CY-505	Advanced inorganic chemistry	3	CY-571	Electives for ***6 credits*** from:	6
CY-506	Organic chemistry lab: Synthesis	3	to	(See titles in the Syllabus)	
CY-507	Instrumentation and computer applications lab	3	CY-582		

Course Code : FN-106
Title of the Course : Symmetry and mathematics

L-T-P : L ~~/ T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): basic graduation level knowledge of mathematics expected but not mandatory.

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : understand basic and different areas of mathematics.

CLO-2 : nurture a mathematical aptitude, thinking, and inculcate skills to solve problems.

CLO-3 : inculcate mathematical reasoning and enable them to understand the mathematical models in chemistry.

CLO-4 : prepare the students to apply the mathematics knowledge in learning and understanding other courses in physical and inorganic chemistry better, especially like quantum chemistry and molecular spectroscopy etc.

CLO-5 : learn the basics of group theory and its application in chemistry. This knowledge may equip them to learn other courses in M.Sc. Chemistry like spectroscopy and coordination chemistry etc.

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	2	2	2	1	3
CLO-2	3	3	3	2	2	2	1	3
CLO-3	3	3	3	2	2	3	1	3
CLO-4	3	3	3	3	2	3	1	3
CLO-5	3	3	2	3	3	3	1	3

Detailed Syllabus (FN-106)

Symmetry elements and operations, point groups. Matrix representation of symmetry operations-Great Orthogonality Theorem-Character tables. Direct product representations. Projection operators and symmetry adapted linear combinations. Applications.

Numbers: Real and Complex number algebra. Vector algebra.

Functions & Variables : Differential calculus-first- and higher-order derivatives, evaluation of minimum and maximum, limits & continuity. Partial differentiations. Exact and inexact differentials. Numerical differentiation. The gamma and delta functions.

Integral Calculus: Indefinite and definite integrals, improper integrals. Methods of integration. Surface and volume integrals. Numerical integrations.

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.

Matrices and Determinants. Eigenvalues and eigenvectors. Orthogonal transformation. Rank & inverse of matrix.

Solution of Linear Systems: Gaussian elimination, Cramer's rule. Gauss-Jordan elimination. Gauss-Seidel and Jacobi methods. Solution of non-Linear Systems: Newton-Raphson method. Curve fittings.

Probability and Statistics: Permutation & Combination. Probability. Stirling's approximation. Lagrange multipliers.

Suggested reading:

1. Molecular Symmetry and Group Theory. Allan Vincent, John Wiley & Sons, LTD.
2. Symmetry: An introduction to group theory and its applications. R. McWeeny, Dover Publications, Inc.
3. Chemical Applications of Group Theory. F. A. Cotton, John Wiley & Sons, Inc.
4. Symmetry and Structure. S. F. A. Kettle, Wiley.
5. Mathematics for Physical Chemistry. R. G. Mortimer, Academic Press.
6. Advanced Engineering Mathematics. E. Kreyszig, Wiley.
7. Mathematics for Chemistry and Physics. G. Turrell, Academic Press.
8. Numerical Analysis: A Practical Approach. Melvin J. Maron, Macmillan Publishing Co., Inc. NY & Collier Macmillan Publishers, London.

Course Code : CY-401
Title of the Course : Basic Concepts and Coordination Chemistry (3 credits)

L-T-P : L / ~~T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): NIL

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : understand the basics of inorganic and coordination chemistry

CLO-2 : understand and analyse inorganic reaction pathways using redox data

CLO-3 : understand and analyse structure-property correlation of coordination compounds

CLO-4 : design new coordination compounds based on a fundamental understanding of their electronic properties

CLO-5 : appreciate specialized and advanced topics in inorganic and coordination chemistry.

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	2	2	1	3	3
CLO-2	3	3	3	2	3	2	1	3
CLO-3	3	3	3	2	2	1	1	3
CLO-4	3	3	3	2	3	2	2	3
CLO-5	3	3	3	3	3	3	2	3

Detailed Syllabus (CY-401)

Shapes of Small Molecules: VSEPR theory - Coordination polyhedra - Enumeration of geometrical and optical isomers. (3 h)

Theory of Acids and Bases: Bronsted and Lewis acids and bases - Gas phase versus solution acidity - Solvent leveling effects - Hardness and softness - Surface acidity. (5 h)

Oxidation and Reduction: Use of redox potential data - Nernst equation - Influence of complex formation, precipitation, change of pH and concentration on redox potentials - Analysis of redox cycles - Redox stability in water - Disproportionation/Comproportionation - Frost, Latimer and Pourbaix diagrams. (6 h)

Coordination Chemistry: d-orbital splitting in various fields – Spectroscopic states and term symbols - Hole formalism - Tanabe-Sugano and Orgel diagrams - Derivation of Ligand field parameters (Dq. B) from electronic spectra - Magnetic moments - Orbital contribution, spin-orbit coupling and covalency - Molecular orbitals and energy level diagrams for common symmetries - Bonding involving pi-donor ligands - Back-bonding - f-orbital splitting - Spectral and magnetic properties of f-block elements.
(18 h)

Inorganic Reaction Mechanisms: Substitution reactions - Dissociative and associative interchange - trans -effect - Linear free energy relations - Rearrangements - Berry pseudo rotation - Electron transfer reactions - Photo-dissociation, -substitution and -redox reactions, Fluxional molecules. (8 h)

Suggested reading:

(1) P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong: Shriver and Atkins' Inorganic Chemistry, Fifth Edition, 2009, OUP or D. F. Shriver and P. W. Atkins, ''Inorganic Chemistry'', 3rd Edn, OUP, 1999.
(2) C. Housecroft, A. G. Sharpe, ''Inorganic Chemistry'', 3rd Edn, (or 4th Edn in 2012) Prentice Hall/Pearson, 2008.
(3) F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn, John Wiley, 1988 (or F. A. Cotton , C. A. Murillo, M. Bochmann and R. N. Grimes, ''Advanced Inorganic Chemistry'', 6th Edn Wiley, 1999).
(4) J. E. Huheey, E. A. Keiter, R. L. Keiter, ''Inorganic Chemistry: Principles of Structure and Reactivity'', 4th Edn, Prentice Hall, 1997 (or a previous edition).
(5) G. L. Miessler, D. A. Tarr, ''Inorganic Chemistry'', 3rd Edn, Pearson Education, 2004.
(6) G. Wulfsberg, ''Inorganic Chemistry'', University Science Books, 2000.

Course Code : CY-402
Title of the Course : Physical Organic Chemistry

L-T-P : L ~~/ T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): BSc Organic Chemistry

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : Provide insight into physical concepts of structure and bonding

CLO-2 : Appreciate the basic concepts related to the structure and reactivity

CLO-3 : Provide insight into aromaticity

CLO-4 : Discussion and predicting the reactivity based on physical concepts

CLO-5 : Detailed discussion and understanding of stereochemistry and synthesis

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	2	3	1	1	3
CLO-2	3	3	3	2	3	1	1	3
CLO-3	3	3	3	2	2	1	1	2
CLO-4	3	3	3	2	3	3	2	3
CLO-5	3	3	3	3	3	3	2	3

Detailed Syllabus (CY-402)

Structure and bonding: Description of molecular structure using valence bond concept (Hybridization, bond lengths and angles). **[2 h]**

M.O. and V.B. methods (Huckel's MO Method, pictorial representation of MOs for molecules, Qualitative application of MO theory to reactivity). **[5 h]**

Inductive, resonance, hyperconjugation and field effects, hydrogen bonding. **[2 h]**

Aromaticity and Huckel's rule (energy, structural, electronic criteria for aromaticity and relationship among them, aromaticity for annulenes, charged rings, homoaromaticity, fused rings, heteroaromaticiy). **[4 h]**

Thermodynamics and kinetics: Acids and bases, HSAB principle, bond energies and thermochemistry, kinetic parameters, Hammond's postulate, Kinetic isotope effects, kinetic and thermodynamic control (general relationship between thermodynamic stability and reaction rate).

[7 h]

Linear free energy relationships for substituent effects (numerical expression and application to characterization of reaction mechanisms). **[4 h]**

Stereochemistry: Chirality and isomerism in organic systems, resolution and asymmetric synthesis, conformational analysis of acyclic and cyclic systems, Curtin-Hammett principle. Effect of Conformation on reactivity: stereo electronic effects. **[10 h]**

Supramolecular chemistry: Host-guest systems, crowns, cryptands, clathrates and inclusion complexes. **[2 h]**

Reading material

1. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Structure and Mechanisms, Part A, 5th Edition, Springer, 2007.
2. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry Illustrated Edition, University Science, 2005.
3. M. B. Smith and J. March, March Advanced Organic Chemistry, 6th edition, Wiley, 2007.
4. A. J. Kirby, Stereoelectronic Effects, Oxford University Press, 1996.
5. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th edition, Pearson Education.
6. Ian Fleming, Molecular Orbitals and Organic Chemical Reactions-Student Edition, Wiley, London, 2009.
7. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds Wiley Student Edition, 2008.

Web resource: http://chemistry.uohyd.ac.in/~CY402/

Course Code : CY-404
Title of the Course : Inorganic Chemistry Lab: Quantitative and Qualitative Analysis

L-T-P : ~~L / T~~/-P
Credits : 0– 0 –3

Prerequisite Course / Knowledge (If any): Basics of Chemistry (undergraduate)

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: analyze common chemicals for their identity and composition

CLO-2: appreciate the strengths and limitations of various physical techniques to analyze chemicals

CLO-3: have hands-on experience/practical knowledge in performing experiments

CLO-4: separate different metal ions on the basis of their reactivity by checking the reactivity

CLO-5: design/modify the existing set up for chemical analysis

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	1	2	1	3	2	2	2
CLO-2	2	2	2	1	2	1	2	2
CLO-3	3	2	2	2	1	2	2	3
CLO-4	3	2	2	2	2	2	2	3
CLO-5	2	3	3	2	2	2	2	3

Detailed Syllabus (CY-404)

Quantitative Analysis
Statistical analysis of data sampling methods.
Redox titrations (permanganometry, dichromatometry, iodometry).
Complexometric titrations using EDTA (estimation of some metal ions, hardness of water).
Precipitation titration (estimation of Ag).
Quantitative separation of metal ions from a binary mixture (e.g. Cu2+/Fe3+).
Gravimetric analysis (e.g. estimation of Ni2+).
Analysis of ores and minerals (e. g. Iron ore, Potassium alum).
Ion exchange separation of metal ions (e.g. Zn2+/Mg2+).
Ion exchange separation of oxidation states (e.g. VO3□ /VO2+).
Qualitative Analysis
Reactions of some less common metal ions (TI, W, Mo, V, Zr, Th, U).
Simple reactions to illustrate the aqueous chemistry of some typical transition metal ions - several oxidation states of V, Cr, Mn - oxoions - Peroxo ions; complex formation of Co2+ - H2O-HCl reaction.
Group separation of cations (mostly trace elements).

Suggested reading:

(1) Vogel's Textbook of Quantitative Chemical Analysis, 5th Edn, Orient Longman, 1989.
(2) Vogel's Textbook of Macro and Semimicro Qualitative Inorganic Analysis, 5th Edn, Orient Longman, 1982.

Course Code : CY-405
Title of the Course : Organic Chemistry Lab - Techniques

L-T-P : ~~L / T~~ / P
Credits : 0 – 0 – 3

Prerequisite Course / Knowledge (If any): None

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to …

CLO-1 : determine the melting point of pure organic solids

CLO-2 : purify impure organic solids by recrystallization or sublimation

CLO-3 : purify/separate organic liquids by simple and fractional distillation

CLO-4 : verify the purity of organic compounds/identify the number of organic compounds in a mixture employing thin layer chromatography

CLO-5 : purify/separate organic compounds by column chromatography

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	2	2	3	2	1	1	3
CLO-2	3	3	3	3	2	1	1	3
CLO-3	3	3	3	3	2	1	1	3
CLO-4	3	3	3	3	2	1	1	3
CLO-5	3	3	3	3	2	1	1	3

Detailed Syllabus (CY-405)

Different laboratory techniques-melting point, distillation, thin layer chromatography (TLC), column chromatography, sublimation, crystallization.
Separation and analysis of organic compounds.

Suggested Reading:

1. A.I. Vogel, Textbook of Practical Organic Chemistry, 4th edition.
2. Laboratory manual.

Course Code : CY-406
Title of the Course : Computer Programing Laboratory

L-T-P : L ~~/ T~~ / P
Credits : 0.5 – 0 – 1.5

Prerequisite Course / Knowledge (If any): NONE

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to …

CLO-1: understand Linux operating system, Linux commands, usage of computer programing in numerical analysis.

CLO-2: understand the concept of Fortran (F77) programming, syntax of Fortran program; declaration of variables, character declaration, numeric precision, input/output statements, operators, if-else-constructs, do-loops, arrays

CLO-3: appreciate basic numerical algorithms

CLO-4: apply Fortran programming to write algorithms for simple problems like sorting a large set of number, matrix addition/multiplication, integration, algebraic equations

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	1	3	1	1	3	3	3
CLO-2	3	1	3	1	1	3	3	3
CLO-3	3	1	3	1	1	3	3	3
CLO-4	3	1	3	1	1	3	3	3

Detailed Syllabus (CY-406)

Unit 1: Programming Laboratory (Linux OS, vi editor)

Unit 2: Programming in FORTRAN

Unit 2: Examples of numerical algorithms – algebraic equations, numerical integration, curve fitting, matrix computations

Unit 3: Students are instructed to write FORTRAN programs on some of the numerical methods taught.

Suggested reading:

1. Numerical Analysis and Computational Programming, S. A. Mollah, Books and Allied (P) Ltd.

2. Fortran 77 and Numerical Methods, C. Xavier, New Age International Publishers.

3. Computer Programming in Frotran, V. Rajaraman, PHI Learning Private Limited.

4. Numerical Recipes in Fortran: The art of Scintific Computing, W. H. Press, S. A. Teukolsky, W. T. Vellerling and B. P. Flannery, Cambridge University Press

Course Code : CY-451
Title of the Course : Main Group and Inner Transition Elements

L-T-P : L ~~/ T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): MSc course CY401

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: analyze the position, periodicity and properties of main group elements and inner transition elements.

CLO-2: comprehend why elements behave the way they do and analyzing the apparent anomalies

CLO-3: get information on new reactions and pathways for future uses, if any

CLO-4: search the literature through textbooks or e-resources on the subject

CLO-5: appreciate advanced topics in the subject for future applications

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	2	1	3	3	1	1	1	2
CLO-2	3	1	3	2	1	2	2	3
CLO-3	3	2	3	2	2	2	2	3
CLO-4	2	2	3	2	1	1	2	3
CLO-5	2	3	2	2	1	2	1	3

Detailed Syllabus (CY-451)

Perspectives, periodicity & periodic anomalies – Relativistic effects on chemical properties (2 h)

Hydrogen and its compounds: H-bond and its influence on the structure and properties of crystals- Hydrides→classification: electron deficient, electron precise and electron rich hydrides (2 h)

Alkali and alkaline earth metals: Solutions in liquid ammonia - Synthesis, properties, uses and structures of crown ether complexes, cryptands and organometallic compounds (2 h)

Group 13 elements: Borides, borates, boron halides, boranes, carboranes and metallocarboranes, BN compounds, transition-metal stabilized borylene and boryllithium, organoaluminum compounds, Lewis Base adducts of AlR3 compounds, Subvalent organo-Al compounds, Organo-gallium, -indium, and –thallium compounds (8 h)

Group 14 elements: Allotropes of Carbon- C60 and its compounds (fullerenes) - carbon nanotubes: synthesis and properties -Intercalation compounds of graphite - Pure Silicon, silica and silicates, Silicones - Low coordinated and hypervalent Silicon compounds - Brief survey of Ge, Sn, and Pb chemistry- Organo-germanium, -tin, and -lead compounds (6 h)

Group 15 elements: P(V) compounds (structure, bonding, reactivity) - P(III) compounds: diphosphenes, phosphaalkenes, iminophosphanes - P-containing ring systems (phosphabenzene, phosphole), phosphazenes, P-S compounds (7 h)

Group 16 elements: Sulfur - polycationic and anionic species - SN compounds.(3 h)

Group 17 elements: Charge-transfer complexes of halogens, interhalogen compounds, halogen oxides and oxygen fluorides, pseudohalogens. (3 h)

Group 18 elements: Noble gas clathrates and compounds. (3 h)

Inner transition elements: Chemistry of f-block elements - Binary compounds - Organometallic compounds - Relation to p-block and d-block chemistry - Transactinides (super-heavy elements). (4 h)

Suggested reading:

(1) A. G. Massey, "Main group chemistry", Wiley, 2000.
(2) N. N. Greenwood and A. Earnshaw, "Chemistry of the Elements", Pergamon Press, 1989.
(3) P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong: Shriver and Atkins' Inorganic Chemistry, Fifth Edition, 2009, OUP or D. F. Shriver and P. W. Atkins, ''Inorganic Chemistry'', 3rd Edn, OUP, 1999.
(4) C. Housecroft, A. G. Sharpe, ''Inorganic Chemistry'', 3rd Edn, (or 4th Edn in 2012) Prentice Hall/Pearson, 2008.
(5) F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn, John Wiley, 1988 (or F. A. Cotton , C. A. Murillo, M. Bochmann and R. N. Grimes, ''Advanced Inorganic Chemistry'', 6th Edn Wiley, 1999).
(6) J. E. Huheey, E. A. Keiter, R. L. Keiter, ''Inorganic Chemistry: Principles of Structure and Reactivity'', 4th Edn, Prentice Hall, 1997 (or a previous edition).

Course Code : CY-452
Title of the Course : Organic Reactions and Mechanisms

L-T-P : L ~~/ T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): Basic and physical organic chemistry

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : understand the basics of reaction intermediates

CLO-2 : understand the insights of the reaction mechanism.

CLO-3 : understand the oxidation and reduction of organic chemistry.

CLO-4 : understand the detailed photochemical reactions and cyclization process.

CLO-5 : understand the impact of heterocycles in organic synthesis.

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	2	2	2	2	2	2	3
CLO-2	3	2	3	2	3	2	2	3
CLO-3	3	3	2	2	2	3	1	3
CLO-4	3	3	3	3	3	3	3	3
CLO-5	3	3	2	3	3	3	3	3

Detailed syllabus (CY-452)

Methods of formation, structure determination and reactions of the following reactive intermediates: carbocations, carbanions, free radicals, carbenes and nitrenes, arynes and related species. [5 h]

Detailed reaction mechanisms and effect of different parameters in the regio-, stereo-, chemo-selective outcome of addition, substitution, elimination, oxidation, reduction, rearrangement and pericyclic reactions. [22 h]

Baldwin ring closure rules, formation of 3,4,5 and 6 membered rings. [2 h]

Reactions of aromatic heterocycles: Synthesis and properties. [4 h]

Organic photochemical reactions. [3 h]

Suggested Text Books:

1. M. B. Smith and J. March, March Advanced Organic Chemistry, 6th edition, Wiley, 2007.
2. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Structure and Mechanisms, Part A, 5th Edition, Springer, 2007.
3. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 1st edition, Oxford University Press, 2001.
4. K. Peter C. Vollhardt and N. E. Schore, Organic Chemistry, W. H. Freeman and Company, 1999.
5. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th edition, Pearson Education.
6. Ian Fleming, Molecular Orbitals and Organic Chemical Reactions-Student Edition, Wiley, London, 2009.
7. J. D. Coyle, Introduction to Organic Photochemistry, Wiley, 1991.
8. B. Halton, J. M. Coxon, Organic Photochemistry, Cambridge University Press, 2011.
9. S. Sankararaman, Pericyclic Reactions: A Textbook: Reactions, Applications and Theory, Wiley-VCH, 2005.

Course Code : CY-453
Title of the Course : Molecular Spectroscopy

L-T-P : L ~~/ T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): FN-106, CY-403

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : understand the basic principles of light-matter interactions and learn quantum mechanical methods to analyze the interactions

CLO-2 : apply quantum mechanical methods to obtain selection rules and spectra of di- and poly-atomic molecules in microwave, infrared, Raman, UV-Vis spectroscopy

CLO-3 : learn various spectroscopic methods based on the magnetic resonance principles

CLO-4 : analyze spectroscopic information to obtain structural information of molecules

CLO-5 : learn principles of XPS and EPR spectroscopy to analyze the elemental composition, chemical bonding characteristics and radical nature of a sample

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	2	3	2	1	3
CLO-2	3	3	3	2	3	2	1	3
CLO-3	3	3	3	2	3	2	1	3
CLO-4	3	3	3	2	3	2	1	3
CLO-5	3	3	3	2	3	2	1	3

Detailed Syllabus (CY-453)

Interaction of radiation with matter, semiclassical treatment. Time-dependent perturbation theory and transition rates. Electric dipole, quadrupole and magnetic dipole transitions. Selection rules. Line width and line shapes.

Rotational, vibrational and ro-vibrational spectroscopy of di-atomic molecules. Selection rules. Rotational energy levels of polyatomic molecules. Classification of rotors and selection rules. Applications. Polyatomic molecular vibrations. Local and normal modes. Infrared spectroscopy, selection rules. Rotational and vibrational Raman Spectroscopy and selection rules.

Franck-Condon principle. Electronic spectroscopy. Selection rules. Resonance Raman transitions and application. Radiative and nonradiative decay- internal conversion and intersystem crossing. Principles of Laser.

Electron Spectroscopy- PES, XPS and ESCA.

NMR spectroscopy-origin of chemical shift and spin-spin coupling. AX, AX2 and AXn systems. Paramagnetic shifts and their applications. Introduction to relaxation processes in solution.

EPR spectroscopy-relaxation processes. Origin of g-shifts and hyperfine coupling. Negative spin densities. Experimental determination of g, A and D tensors-their interpretation with examples.

Principles of Mossbauer spectroscopy. Origin of isomer shifts, quadrupole splitting and h. f. s.

Suggested reading:

1. Molecular Spectroscopy. I. N. Levine, Wiley –Interscience Publication.
2. Molecular Spectroscopy. J. D. Graybeal,McGraw Hill.
3. Modern Spectroscopy. J. M. Hollas, John Wiley & Sons.
4. High Resolution Spectroscopy. J. M. Hollas, Butterworths.
5. Fundamentals of Molecular Spectroscopy. C. N. Banwell and E. M. McCash, Tata McGraw-Hill publishing.
6. Principles of Ultraviolet Photoelectron Spectroscopy, J. W. Rabalais, John Wiley & Sons.
7. Molecular Spectra & Molecular Structure. G. Herzberg, Van Nostrand Reinhold Company.

Course Code : CY-454
Title of the Course : Chemical and Statistical Thermodynamics

L-T-P : L ~~/ T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): FN-106, CY-151, CY-403

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : discuss the principles of energy conservation, direction of flow of energy and direction of chemical reactions

CLO-2 : comprehend the concepts disorderedness in connection to the equilibrium properties of the system

CLO-3 : appreciate and develop the tools of statistical mechanics to systems under different conditions

CLO-4 : analyze of the connection of microscopic details of constituent molecules to the macroscopic properties of a system

CLO-5 : apply of tools and methods of equilibrium statistical mechanics to understand and analyze various properties of chemical systems

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	2	2	3	2	3
CLO-2	3	3	3	2	2	3	2	3
CLO-3	3	3	3	2	2	3	2	3
CLO-4	3	3	3	2	2	3	2	3
CLO-5	3	3	3	2	2	3	2	3

Detailed Syllabus (CY-454)

Review of classical thermodynamics. Mathematical apparatus.

Concepts of statistical thermodynamics. Micro canonical, canonical and grand canonical ensembles. Ensemble averages. Most probable distribution. Undetermined multipliers. Fluctuations.

Boltzmann statistics, Fermi-Dirac statistics and Bose-Einstein statistics.

Ideal monatomic, diatomic and polyatomic gas. Partition functions.

Equilibrium constant in terms of partition functions, Debye-Hückel theory. Statistical mechanics of ionic solutions. Flory-Higgins theory of polymer solutions. Specific heats of solids- Einstein and Debye models.

Virial equation of state and virial coefficients. The law of corresponding states. Elementary kinetic theory of transport in gases.

Suggested reading:

1. Physical Chemistry. P. W. Atkins and J. de Paula, Oxford University Press.
2. Physical Chemistry. I. N. Levine, McGraw Hill.
3. Physical Chemistry. R. G. Mortimer, Academic Press.
4. Statistical Mechanics. D. A. McQuarrie, University Science Books.

Course Code : CY-455
Title of the Course : Biological Chemistry

L-T-P : L / ~~T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): None

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to …

CLO-1 : identify various classes of biomacromolecules and their building blocks

CLO-2 : appreciate the basic principles that govern the three-dimensional structures adopted by different classes of biomolecules

CLO-3 : understand the flow of information from genetic material to proteins and other biomolecules

CLO-4 : derive structure-function correlations for various classes of biomolecules

CLO-5 : appreciate that metabolic pathways which regulate biological processes basically involve chemical reactions mediated by enzymes and other biomolecules

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	1	2	2	1	1	1	3
CLO-2	3	2	3	3	2	1	1	3
CLO-3	3	3	3	3	2	1	1	3
CLO-4	3	3	3	3	2	1	1	3
CLO-5	3	3	3	3	2	1	1	3

Detailed Syllabus (CY-455)

Cell Structure and Function: Structure of prokaryotic and eukaryotic cells, intracellular organelles and their function, comparison of plant and animal cells.

Introduction to biomolecules: Examples of biomolecules and building blocks of biopolymers. Types of reactions occurring in cells, structure of ice and liquid water, hydrogen bonding and hydrophobic interactions, buffers and the Henderson-Hasselbalch equation.

Amino acids, peptides and proteins: Primary structure of proteins, end group determination, amino acid analysis and the Edman degradation (protein sequencing), Ramachandran plot and the secondary structure of proteins α-helix, β-pleated sheet, β-bend and collagen triple helix. Tertiary structure and structural motifs - protein folding and domain structure of proteins. Oligomeric proteins. Purification and characterization of proteins, functions of proteins.

Enzymes and catalysis: Substrate specificity of enzymes, requirement of coenzymes, regulation of enzyme activity and allosteric effect, enzyme nomenclature, enzyme kinetics and the Michaelis-Menten equation, various types of enzyme inhibition. application of enzymes in chemical synthesis, enzyme models and their applications.

Nucleotides and nucleic acids: Ribonucleotides and deoxyribonucleotides, RNA and DNA. Base pairing, double helical structure of DNA and forces stabilizing nucleic acid structure. Methods used in nucleic acid separation and characterization, nucleic acid sequencing.

Transcription and translation: Messenger RNA, RNA polymerase and protein synthesis. Control of transcription and protein-DNA interactions. The genetic code, tRNA structure and codon-anticodon interactions. Ribosomes and their structure. Gene cloning and site-directed mutagenesis.

Carbohydrates: Monosaccharides, oligosaccharides and polysaccharides, carbohydrates of glycolipids and glycoproteins, role of sugars in biological recognition, blood group substances.

Lipids and membranes: Common classes of lipids - glycerolipids, phospholipids, sphingolipids and glycolipids. Self-association of lipids - formation of micelles, reverse micelles and membranes, gel and liquid-crystalline phases. Lipid phase polymorphism - bilayer, hexagonal and cubic phases. Liposomes and their properties and applications. Biological membranes and the fluid mosaic model, current models of biological membranes, membrane proteins and their functions, membrane asymmetry.

Introduction to metabolism: Overview of metabolism, catabolic and anabolic processes, glycolysis, citric acid cycle and oxidative phosphorylation.

Suggested reading:

1. Biochemistry by *D. Voet & J. G. Voet*, 4th Edition (2010) Published by John Wiley (New York).
2. Lehninger's Principles of Biochemistry by *D. L Nelson & M. M. Cox*, 5th Edition (2008) Published by W. H. Freeman (New York) and CBS Publishers (New Delhi).
3. Biochemistry by *J. M. Berg, J. L. Tymoczko & L. Stryer*, 5th Edition (2002) Published by W. H. Freeman (New York).

Course Code : CY-456
Title of the Course : Inorganic Chemistry Lab: Synthesis

L-T-P : ~~L / T~~ / P
Credits : 0 – 0 – 3

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: provide basic principles of inorganic synthesis

CLO-2: understand the strategies for synthesis of various types of inorganic compounds

CLO-3: analyze and interpret physical properties in relation to the structure of the compound

CLO-4: design and execute a strategy for synthesis of a given compound

CLO-5: to synthesize and characterize a new compound

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	3	2	1	1	3
CLO-2	3	3	3	2	2	1	1	3
CLO-3	3	3	3	2	2	1	1	3
CLO-4	3	3	3	2	3	3	2	3
CLO-5	3	3	3	3	3	3	2	3

Detailed syllabus (CY-456)

Synthesis of a variety of Inorganic Compounds/Complexes of 3d metal ions, main group elements and rare earths by using common experimental techniques.

Introduction to various physical measurements (IR, UV-Vis, Mass, NMR, Magnetic susceptibility, EPR and X-ray diffraction) for characterization of the compounds.

Analysis and interpretation of the physical data of the compounds to determine their structures.

Study of the related literature.

Preparation of Scientific Reports.

Course Code : CY-501
Title of the Course : Spectroscopic Methods for Structure Elucidation

L-T-P : L ~~/ T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): A course on Molecular Spectroscopy (Physical Aspects)

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : understand the basics of different spectroscopic techniques (UV, Mass, IR and NMR).

CLO-2 : understand specialized and advanced spectroscopic experiments for the structural elucidation of organic compounds.

CLO-3 : do structural elucidation of unknown organic compounds using combined spectral data.

CLO-4 : design different spectroscopic experiments to address the regio and stereo chemical outcome in products of an organic reaction.

CLO-5 : apply different spectroscopic techniques to address the day to day societal needs.

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	2	2	2	1	2	1	3
CLO-2	3	2	2	2	1	2	1	3
CLO-3	3	3	2	2	1	3	1	3
CLO-4	3	3	3	3	3	3	3	3
CLO-5	3	3	2	3	3	3	3	3

Detailed syllabus (CY-501)

NMR Spectroscopy: **[16 h]**

^{1}H NMR, Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift □, inductive and anisotropic effects on □, chemical structure correlations of □, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant J, first order patterns. Second order effects, examples of AB, AX and ABX systems, simplification of second order spectrum, selective decoupling, use of chemical shift reagents for stereochemical assignments. ^{13}C NMR, introduction to FT technique, relaxation phenomena, NOE effects, ^{1}H and ^{13}C chemical shifts to structure correlations. Study of dynamic processes by VT NMR, restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (bullvalene and related systems). 2D NMR spectroscopy. Multinuclear NMR.

Electronic spectroscopy: **[3 h]**

Basic principle, electronic transitions and application to structure elucidation.

Polarimetry: **[1 h]**

Optical rotatory dispersion and circular dichroism.

Infrared Spectroscopy: **[5 h]**

Organic functional group identification through IR spectroscopy.

Mass spectrometry: **[6 h]**

Basic principles, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution MS, soft ionization methods, ESI-MS and MALDI-MS, illustrative examples from macromolecules and supramolecules.

Structure elucidation problems using the above spectroscopic techniques. **[6 h]**

Suggested Text Books:

1. R. M. Silverstein, F. X. Webster, D. J. Kiemle, Spectrometric identification of organic compounds, 7th edition, John Wiley, 2005.
2. Organic Spectroscopy, W. Kemp, 3rd edition, Macmillan, 2011.
3. D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, McGraw Hill, 6th edition 2007.
4. D. L. Pavia and G. M. Lampman Spectroscopy 4th Edition, Brooks Cole, 2012.
5. H. Gunther, NMR Spectroscopy Wiley-VCH, 2013.
6. P. S. Kalsi, Spectroscopy of Organic Compounds, 6th edition, New age international, 2004.

Course Code : CY-502
Title of the Course : Advanced Organic Synthesis

L-T-P : L / ~~T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): M.Sc courses in I – II semesters

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: understand different types and distinctive features of advanced organic reactions and reagents

CLO-2: understand the advanced concepts related to the structure and properties of various organic reagents, catalysts and compounds

CLO-3: understand and analyze the structure, reactivity and properties of pharmaceutical drugs to natural organic compounds

CLO-4: design new catalysts, new reactions and properties based on the fundamental insights received about the molecules

CLO-5: appreciate the advanced sustainable reactions and catalysts for revolutionary applications

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	3	3	2	2	3
CLO-2	3	3	3	3	3	2	2	3
CLO-3	3	3	3	3	3	2	2	3
CLO-4	3	3	3	3	3	2	2	3
CLO-5	3	3	3	3	3	2	2	3

Detailed Syllabus (CY-502)

Synthetic analysis and Planning: Retrosynthetic analysis, synthetic equivalent, control of stereochemistry, linear, convergent and divergent syntheses. (4 h)

Use of protecting groups in multi-step synthesis: Different protection and deprotection methods. (3 h)

Modern synthetic methods involving various oxidizing, reducing agents, C-C bond forming reactions by alkylation, acylation, organometallic, radical, pericyclic reactions and rerrangements. Discussion of selected syntheses of natural products/bioactive molecules/organic materials. (24 h)

Organocataytic transformations and C-H activation reactions-selected examples. Solid phase organic synthesis. (3 h)

Atom economy, step economy and green chemistry and environmental aspects. (2 h)

Suggested reading:

1. G. S. Zweifel and M. H. Nantz, *Modern Organic Synthesis-An Introduction*, W. H. Freeman and Company, 2006.

2. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry*, Part B, Fifth Edition, 2007

3. E. J. Corey and X. M. Cheng, *The Logics of Chemical Synthesis*, Wiley, 1989.

4. K. C. Nicolaou, *Classics in Total Synthesis*, Vol 1, 2 and 3.

5. S. Warren and P. Wyatt, *Organic Synthesis: The Disconnection Approach*, 2nd edition, Wiley, 2008.

6. J. H. Fuhrhop, G. Li, *Organic Synthesis: Concepts and Methods*, 3rd edition, VCH, 1994.

7. W. Carruthers, *Some Methods of Organic Synthesis*, Cambridge University Press.

8. H. O. House, *Modern Synthetic Reactions*, Benjamin-Cummings Publishing Co. 1972.

Course Code : CY503
Title of the Course : Chemical Dynamics

L-T-P : L / ~~T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): MSc courses in I and II semesters

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : understand the various kinetic parameters, their measurements and utilities

CLO-2 : obtain theoretical understanding of how chemical reactions take place.

CLO-3 : learn experimental techniques for measuring the kinetics of fast reactions, homogeneous and heterogeneous catalyzed reactions.

CLO-4 : appreciate the theoretical and experimental developments in molecular reaction dynamics

CLO-5 : obtain an understanding of various transport properties in gas and solution phase.

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	2	2	2	2	2	2	2	2
CLO-2	3	3	2	2	2	2	2	2
CLO-3	3	3	3	3	3	3	3	2
CLO-4	3	3	3	3	2	2	2	2
CLO-5	3	3	3	3	3	3	3	3

Detailed Syllabus (CY-503)

1. Review of basic concepts in kinetics
2. Fast reactions: experimental techniques
3. Theories of reaction rates
4. Unimolecular reactions
5. Reactions in solution: reactions between ions, diffusion-controlled reactions, electron transfer reactions
6. Composite reactions including photochemical reactions
7. Homogeneous and heterogeneous catalysis
8. Kinetic isotope effect
9. Molecular reaction dynamics
10. Transport properties: Diffusion, viscosity, thermal conductivity, ion transport, dynamic electrochemistry

Suggested reading:

1. Physical Chemistry: A Molecular Approach. D. A. McQuarrie and J. D. Simon, University Science books
2. Physical Chemistry. P. W. Atkins and J. de Paula, Oxford University Press.
3. Physical Chemistry. I. N. Levine, McGraw Hill.
4. Chemical Kinetics. K.J. Laidler, Pearson.
5. Chemical Kinetics and Reaction Dynamics, P.L. Houston, Dover Publications, 2006

Course Code : CY-504
Title of the Course : Chemical Binding

L-T-P : L / ~~T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): FN106, CY403, CY453

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : acquire fundamental understanding of structure and bonding in chemistry

CLO-2 : learn fundamental principles and concepts that leads to different types of chemical bond

CLO-3 : develop concept of molecular orbitals and their experimental manifestation and concept of electronic state

CLO-4 : explain the chemical reactivity based on electronic structure of molecules

CLO-5 : interpret underlying phenomena at a molecular level in all branches of chemistry

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	3	1	2	1	3
CLO-2	3	3	3	2	1	2	2	3
CLO-3	3	2	2	3	1	2	1	3
CLO-4	3	3	2	2	1	2	1	3
CLO-5	3	3	2	3	1	2	1	3

Detailed Syllabus (CY-504)

The Born-Oppenheimer approximation. Electronic structure theory: MO and VB theories, application to H2+ and H2. MO and VB wavefunctions of polyatomic systems. Hückel pi-electron theory. Walsh diagram and molecular geometry.

Hartree-Fock theory, Brillouin conditation, Non-orthogonal basis and Roothaan equation, SCF method. Koopmann's theorem.

Post Hartree-Fock methods. Electron correlation. Basis sets.

Density functional theory and application.

Suggested reading:

1. Quantum Chemistry, H. Eyring, J. Walter and G. E. Kimball, John Wiley & Sons.
2. Quantum Chemistry, D. A. McQuarrie, University Science Books.
3. Quantum Chemistry. I. N. Levine, PHI Learning Private Ltd.
4. Molecular Quantum Mechanics. P. W. Atkins and R. S. Friedman, Oxford University Press.
5. The Chemical Bond, J. N. Murrell, S. F. A. Kettle and J. M. Tedder, John Wiley and Sons.
6. Modern Quantum Chemistry. A. Szabo and N. S. Ostlund.

Course Code : CY-505
Title of the Course : Advanced Inorganic Chemistry

L-T-P : L ~~/ T / P~~
Credits : 3– 0 – 0

Prerequisite Course / Knowledge (If any): Basic inorganic chemistry/spectroscopy courses

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : understand the structure, bonding, reactivity including safe handling of various organometallic compounds

CLO-2 : understand and apply the various organometallic compounds for catalytic applications relevant to chemical and polymer industries.

CLO-3: interpret the structure and function of various elements in biological systems using X-ray diffraction, spectroscopy and magnetic measurement techniques.

CLO-4 : explain the function of various elements in biological systems.

CLO-5 : design and develop new organometallic and bio-inorganic model systems.

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	2	3	1	1	3
CLO-2	3	3	3	2	3	1	1	3
CLO-3	3	3	3	2	2	1	2	3
CLO-4	3	3	3	2	3	3	2	3
CLO-5	3	3	3	3	3	3	2	3

Detailed syllabus (CY-505)

Recent Advances in Main Group Chemistry: Low and hypervalent compounds – p(pi)-p(pi) bonding in heavier main group chemistry. (3 h)

Organometallic Chemistry: Complexes with pi-acceptor and sigma-donor ligands - 16 electron and 18 electron rules – Stability and Reactivity - Isolobal analogy - Structure and bonding - Agostic interaction. (8 h)

Homogeneous and Heterogeneous Catalysis: Hydrogenation, carbonylation, polymerization, Wacker oxidation and other reactions catalyzed by transition metal complexes. (5 h)

Metal Cluster Compounds: Metal-metal bond - Carbonyl and non-carbonyl clusters - Structure and bonding - Low-dimensional solids - Clusters in catalysis. (4 h)

Bioinorganic Chemistry: Biochemistry of iron– its storage, transport and function; Transport and storage of dioxygen– structure and function of haemoglobin, myoglobin, hemocyanin and hemerythrin; Electron transport proteins– cytochromes and Fe-S proteins; Copper containing enzymes– blue and non-blue copper enzymes, ascorbate oxidase, tyrosynase, galactose oxidase, superoxide dismutase; Zinc containing enzymes– carboxy peptidase A, carbonic anhydrase, alcohol dehydrogenase; Iron containing enzymes– catalase, peroxidase and cytochrome P-450; Photosynthesis; Nitrogen fixation; Bioinorganic chemistry of alkali and alkaline earth metal cations; Toxicity of metals. (16 h) Inorganic Photochemistry: Ligand field photochemistry of d^n complexes - Photochemistry of carbonyl compounds - Energy conversion (solar) and photodecomposition of water. (4 h)

Suggested reading:

(1) Textbooks suggested for CY-401.

(2) B. D. Gupta, A. J. Elias, “Basic Organometallic Chemistry”, University Press, 2010.

(3) I. Bertini, H. B. Gray, S. J. Lippard, J.S. Valentine, “Bioinorganic Chemistry”, VLSE with Univ. Sci. Books, 1998

(4) G. L. Miessler, D. A. Tarr, ‘’Inorganic Chemistry’’, 3rd Edn, Pearson Education, 2004.

Course Code : CY-507
Title of the Course : Instrumentation and Computer Applications Lab

L-T-P : ~~L / T~~ / P
Credits : 0 – 0 – 3

Prerequisite Course / Knowledge (If any): A course on basic physics

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to

CLO-1: understand electronic circuits used in spectrometers and research equipment

CLO-2 : have a theoretical and analytical understanding of how spectrometers and research equipment work

CLO-3: carry out minor repair of instruments

CLO-4 : design and fabricate minor equipment for research and analysis

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	2	2	2	2	2	1	1	2
CLO-2	2	2	2	2	3	1	1	2
CLO-3	2	2	2	2	3	1	2	2
CLO-4	2	2	2	2	2	1	1	2

Detailed Syllabus (CY-507)

Instrumentation (electronics)

E1 - Measuring instruments- Introduction to tools and kits; electronic components, mutimeter, potentiometer, decade boxes, power supply, CRO. Simple measurements and cross checks (e.g., resistance read from color codes vs measurement using multimeter)
E2 - (a) Capacitor as charge storage device. Introduction to circuit; kinetics of charging and discharging for several capacitors (b) Measurement of dielectric constant of a solvent (e.g., methanol) by the use of a variable capacitor
E3 - RC, LR, LCR circuits. Concept of filter circuits; determination of cut-off frequency by the use of circuits; frequency selection by the use of LCR circuit; tuning and matching frequencies in NMR and EPR spectrometers by the use of LCR
E4 - Diode characteristics and rectifier circuits. Thermionic emission and VI curve of diodes; measurement of VI curves of diodes including Zener; AC to DC conversion by half-wave and full-wave rectifier circuits; bridge rectification circuit; use of capacitor filters; ripple factor
E5 - Transistor amplifier circuits. Base, emitter and collector in the transistor; forward and reverse bias; soldering the amplifier circuit; voltage amplification by the use of different resistors in the amplifier circuit
E6 - Inverting and non-inverting amplifiers; simple integration and differentiation using operational amplifier
E7 - RS 232 cable and port; computer-instrument interfacing

Computational

C1 - Study of normal modes- optimization of molecular geometry, computation of normal modes and frequencies, analysis of the symmetries of the normal modes, effect of molecular symmetry on the degeneracies, impact of mass on the frequencies
C2 - Determination of equilibrium constants- optimization of molecular geometry of reactant and product, computation of the rotational constants, vibrational frequencies etc., calculation of partition functions, calculation of equilibrium constant at different temperatures
C3 - Determination of rate constants- optimization of molecular geometry of reactant and product, calculation of transition state, computation of the rotational constants, vibrational frequencies etc. for the reactant and transition state, calculation of partition functions, calculation of rates at different temperatures
C4 - Franck-Condon spectral calculations- optimization of the geometry of the ground, excited and ionized excited states, calculation of the vibrational frequencies of these states, calculation of the transition energies and oscillator strengths for the photo-electron spectra
C5 - Construction of Walsh diagram- computation of the MO energies at different geometries of a molecule (eg. H2O, Li2O), examination of the molecular orbitals and their symmetries, plot of the MO energies versus the geometric parameter reactant, qualitative analysis of the trends in the orbital energy variations
C6 - Woodward – Hoffman correlation diagrams- optimization of the geometries of cyclobutene and butadiene, computation of the molecular orbitals and their energies as a function of ring opening of cyclobutene under con- and dis-rotatory modes, plot of the frontier MO energies vs the ring opening coordinate (maintenance of symmetry), analysis of the plots and discussion about thermal / photochemical processes
C7 - Molecular modeling- H-bonded complexes – geometry optimization, analysis of energetics; exciton coupling in chromophore aggregates; effects of solvation
Alternative experiments- Intrinsic reaction coordinate, Natural bond orbital analysis

Course Code : CY-551
Title of the Course : Chemistry of Materials

L-T-P : L ~~/ T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): MSc courses in the I – III semesters

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : provide insight into the various classes and distinct features of materials

CLO-2 : appreciate the basic concepts related to the structure and properties of materials

CLO-3 : understand and analyze the structure-function correlations in materials

CLO-4 : design new materials based on a fundamental understanding of their attributes

CLO-5 : appreciate advanced materials for contemporary and futuristic applications

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	2	3	1	1	3
CLO-2	3	3	3	2	3	1	1	3
CLO-3	3	3	3	2	2	1	1	3
CLO-4	3	3	3	2	3	3	2	3
CLO-5	3	3	3	3	3	3	2	3

Detailed Syllabus (CY-551)

SOLID STATE STRUCTURE [5 h]

Order - spatial, orientational; Types of solids; Symmetry in crystals - primitive lattice vector – Wigner-Seitz cell - crystal systems - Bravais lattices - crystallographic point groups and space groups; X-ray diffraction - reciprocal lattice - Ewald construction - structure factor - systematic absences - crystal structure solution and refinement - common crystal structure motifs; idea of quasicrystals.

DEFECTS AND NONSTOICHIOMETRY [2 h]

Point, line and plane defects; Intrinsic and extrinsic defects - vacancies, Schottky and Frenkel defects - charge compensation; Nonstoichiometry and defects - thermodynamic and structural aspects; Color centres.

THERMAL PROPERTIES [2 h]

Lattice vibrations - phonon spectrum; Lattice heat capacity; Thermal expansion; Thermal conductivity.

ELECTRICAL PROPERTIES [9 h]

Free electron theory - electrical conductivity and Ohm's law - Hall effect; Band theory - band gap - metals and semiconductors - intrinsic and extrinsic semiconductors; Hopping semiconductors; Semiconductor/metal transition; p-n junctions; Superconductors - Meissner effect - type I and II superconductors - isotope effect - basic concepts of BCS theory - manifestations of the energy gap - Josephson devices.

MAGNETIC PROPERTIES [3 h]

Classification of magnetic materials; Langevin diamagnetism; Quantum theory of paramagnetism; Cooperative phenomena - ferro, antiferro and ferrimagnetism - magnetic domains and hysteresis; Superparamagnetism.

OPTICAL PROPERTIES [2 h]

Optical reflectance - plasmon frequency; Raman scattering in crystals; Photoconduction; Photo and electroluminescence; Lasers; Photovoltaic and photoelectrochemical effects.

GENERAL CONCEPTS IN MATERIALS SYNTHESIS [3 h]

Phase diagrams; Preparation of pure materials; Nucleation and crystal growth; Crystal growth techniques; Zone refining.

INTRODUCTON TO DIFFERENT CLASSES OF MATERIALS [14 h]

HIGH T_C MATERIALS

Defect perovskites; High T_C superconductivity in cuprates; Preparation and characterisation of 1-2-3 and 2-1-4 materials; Normal state properties - anisotropy; temperature dependence of electrical resistance - superconducting state; Applications.

IONIC CONDUCTORS

Types of ionic conductors; Mechanism of ionic conduction - interstitial jumps - vacancy mechanism – diffusion; Superionic conductors - phase transitions; Examples and applications of ionic conductors; Fuel cells.

POLYMERS

Molecular shape, structure and configuration; Crystallinity; Mechanical properties - stress-strain behaviour; Thermal behaviour - glass transition; Polymer types and their applications; Conducting, luminescent and ferroelectric polymers.

LIQUID CRYSTALS

Mesomorphic behaviour - thermotropic and lyotropic phases; Ordering in liquid crystals - the director field and order parameters; Nematic and smectic phases - phase transitions; Chiral nematics - cholesteric-nematic transition - optical properties - twisted nematic effect; Structure-phase relations.

THIN FILMS

Preparation techniques - evaporation/sputtering, chemical processes, MOCVD, sol-gel; Langmuir-Blodgett technique; Properties and applications of thin and ultrathin films.

MOLECULAR MATERIALS

Molecular semiconductors and metals; Organic superconductors; Molecular magnetic materials - single molecule magnets; Fullerenes - doped fullerene superconductors. Molecular electronics.

NANOMATERIALS

Preparation techniques; Scanning probe and electron microscopy; Novel physical phenomena in the nano domain – size effects; Electronic, photonic, magnetic and catalytic applications; Nanocomposites; Carbon nanotubes; Graphene; Molecular nanomaterials.

NONLINEAR OPTICAL MATERIALS

Nonlinear optical phenomena - second and third order effects; Molecular hyperpolarisability and second harmonic generation; Materials and structure-property correlations.

Reading material

1. H. V. Keer, Principles of the Solid State

2. L. E. Smart and E. A. Moore, Solid State Chemistry: an Introduction

3. M. T. Weller, Inorganic Materials Chemistry

4. K. J. Klabunde, Nanoscale Materials in Chemistry

5. W. D. Callister, Materials Science and Engineering, An Introduction

6. C. Kittel, Introduction to Solid State Physics

7. Journals like Chemistry of Materials, Journal of Materials Chemistry, Advanced Materials etc..

Web resource: http://chemistry.uohyd.ac.in/~CY551/

Course Code : CY-552
Title of the Course : Seminar Course

L-T-P : L ~~/ T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): MSc courses in the I – III semesters

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: provide basic level of platform for presentation to a large audience

CLO-2: grasp/comprehend the literature, then analyse and summarize it in an effective way.

CLO-3: know recent advances in chemical literature and to write/present the main points succinctly.

CLO-4: analyze different ways of stage presentation and to make clear slides using the power-point

CLO-5: appreciate/apply advanced topics for future application/reference

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	2	2	3	3	2	2	2	3
CLO-2	3	1	2	3	1	2	2	3
CLO-3	2	1	2	3	1	2	2	3
CLO-4	2	1	2	3	2	2	2	3
CLO-5	2	1	2	3	2	2	2	3

Detailed Syllabus (CY-552)

The main objectives of this course are (i) to train the students to read and understand the journal literature and (ii) to improve their communication skills. Each student has to give a seminar (power-point presentation) on a topic based on a review in a chemistry journal that should have appeared during the previous 10 years. Each seminar will be of 30 minutes [20 min (presentation) + 10 min (Q & A)] duration. Students are expected to be active during all the seminars. Each student has to submit an essay based on the topic he/she has chosen which should be consistent with his/her talk. A final written examination based on the seminars presented by the students will be conducted at the end of the course.

Evaluation is done on the basis of oral presentation [60 marks including Q & A], essay [20 marks] and final written examination [20 marks].

Course Code : CY-553
Title of the Course : Project

L-T-P : ~~L / T~~ / P
Credits : 0 – 0 – 3

Prerequisite Course / Knowledge (If any): None

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : understand research problems.

CLO-2 : execute literature search on a research topic.

CLO-3 : design new experiments to address research problems.

CLO-4 : conduct experiments in a scientific way.

CLO-5 : analyze and interpret the results.

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	2	2	3	3	3	3
CLO-2	3	3	3	2	3	3	3	3
CLO-3	3	3	3	2	3	3	3	3
CLO-4	3	3	3	2	3	3	3	3
CLO-5	3	3	3	3	3	3	3	3

Detailed Syllabus (CY-553)

Each students 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. At the end of the project they will submit a report of the work done and make a presentation.

Course Code : CY-571
Title of the Course : Organometallic Chemistry

L-T-P : L ~~/ T / P~~
Credits : 2 – 0 – 0

Prerequisite Course / Knowledge (If any): A course on understanding the basic principles of organometallic chemistry

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : understand the basics of main group chemistry (organolithium/ zinc/ magnesium/ copper/ titanium etc.)

CLO-2 : understand the insights of the organoboron, aluminium, and silicon chemistry.

CLO-3 : understand the chemistry of metal carbonyls/ carbenes/ benzynes/ NHC.

CLO-4 : understand the cross coupling reactions using Pd/Rh/Ru catalysts.

CLO-5 : understand the impact of C-H activations, Au-catalyzed transformations.

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	2	2	2	2	2	2	3
CLO-2	3	2	3	2	3	2	2	3
CLO-3	3	3	2	2	2	3	1	3
CLO-4	3	3	3	3	3	3	3	3
CLO-5	3	3	2	3	3	3	3	3

Detailed syllabus (CY-571)

1) Organometallic Chemistry of Main Group and Transition metals for applications in organic transformations. [4 h]
2) Carbanionic Organometallics: Organolithium, magnesium, zinc , copper and titanium reagents. [4 h]
3) Chemistry of Organoboron, aluminium, silicon and tin compounds. [4 h]
   Organomercurials and organothalium compounds. [1 h]
4) Chemistry of Metal carbonyls: chromium, iron and cobalt carbonyl reagents. [2 h]
5) Metal carbon multiple bonds: carbenes, carbynes, and N-heterocyclic carbenes. [2 h]
6) Chemistry of Metallocenes: Ferrocene and related compounds. [2 h]
7) Organometallic Chemistry of the Noble Metal: Pd, Rh, Ru and Au catalyzed reactions, involving metal catalyzed coupling, C-H activation and metathesis reactions. [5 h]

Suggested Text Books:

1. D. Astruc, Organometallic Chemistry and Catalysis, Springer, 2007.
2. J. F. Hartwig, Organotransition metal chemistry, University Science Books, 2010.
3. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 4th edition, Wiley, 2005.
4. L. S. Hegedus, B. C. G. Soderberg, Transition Metals in the Synthesis of Complex Organic Molecules, University Science Books, 2010.

Course Code : CY-572
Title of the Course : Supramolecular Chemistry

L-T-P : L ~~/ T / P~~
Credits : 3 – 0 – 0

Prerequisite Course / Knowledge (If any): MSc courses in the I – III semesters

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : provide insight into the various supramolecular interactions

CLO-2 : appreciate the basis of supramolecular chemistry in terms of examples from nature

CLO-3 : understand and analyze the structure-function correlations from supramolecular perspective

CLO-4 : apply basic concepts of analytical and spectroscopic methods to understand host-guest chemistry

CLO-5 : apply Self-assembly and crystal engineering approach to understand host-guest chemistry

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	3	3	1	1	3
CLO-2	3	1	2	2	3	1	1	3
CLO-3	3	3	3	3	2	1	2	3
CLO-4	3	3	3	3	3	3	2	3
CLO-5	3	3	3	3	3	2	2	3

Detailed Syllabus (CY-572)

CONCEPTS **[3 h]**

Definition, Development and Classification, Binding Constants, Supramolecular interactions

SUPRAMOLECULAR CHEMISTRY IN LIFE **[3 h]**

Ionophores, Porphyrin and other Tetrapyrrolic Macrocycles, Coenzymes, Neurotransmitters, DNA and Biochemical Self-assembly

CATION BINDING HOSTS **[6 h]**

Podand, Crown Ether, Cryptand, Spherand - Nomenclature, Selectivity and Solution Behaviour. Alkalides, Electrides, Calixarenes, Siderophores

ANION BINDING HOSTS **[3 h]**

Challenges and Concepts, Biological Receptors, Conversion of Cation Hosts to Anion Hosts, Neutral Receptors, Metal-Containing Receptors, Cholapods

ION PAIR RECEPTORS **[2 h]**

Contact Ion Pairs, Cascade Complexes, Remote Anion and Cation Binding Sites, Symport and Metals Extraction

HOSTS FOR NEUTRAL GUEST **[6 h]**

Clathrates, Inclusion Compounds, Zeolites, Intercalates, Coordination Polymers, Guest Binding by Cavitands and Cyclodextrins

CRYSTAL ENGINEERING **[3 h]**

Concepts, Crystal Nucleation and Growth, Understanding Crystal Structures, Polymorphism, Co-crystals

Reading material

1. J. W. Steed & J. L. Atwood (2009), Supramolecular Chemistry, 2nd Edition, John Wiley
2. G.R. Desiraju (1989), Crystal Engineering. The Design of Organic Solids, Elsevier
3. G. R. Desiraju, J. J. Vittal, A. Ramanan (1989), Crystal Engineering -A Textbook, World Scientific-IISc Press
4. Recent papers from journals and reviews and monographs, etc

Course Code : CY-573
Title of the Course : Stereoselective Organic Synthesis

L-T-P : L ~~/ T / P~~
Credits : 2 – 0 – 0

Prerequisite Course / Knowledge (If any): CY-452, CY-502 (or equivalent)

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: understand different types and distinctive features of advanced organic reactions, catalysts and reagents

CLO-2: understand the advanced concepts related to the structure and properties of various organic catalysts, reagents and compounds

CLO-3: understand and analyze the structure, reactivity and properties of catalysts, reagents, pharmaceutical drugs to natural organic compounds

CLO-4: design new catalysts, new reagents, new green reactions and properties based on the fundamental insights received

CLO-5: appreciate the advanced sustainable reactions, reagents and catalysts for revolutionary applications in modern chemical sciences

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	3	3	2	2	3
CLO-2	3	3	3	3	3	2	2	3
CLO-3	3	3	3	3	3	2	2	3
CLO-4	3	3	3	3	3	2	2	3
CLO-5	3	3	3	3	3	2	2	3

Detailed syllabus (CY-573)

Brief review of stereochemistry (1 h)

Chiral pool approach, Acyclic stereoselection: reactions at α-and β–positions of a chiral center. Auxillary econtrolled stereoselection: Evans oxazolidones, Oppolzer sultams, Myers amides, Enders RAMP/SAMP, Shollkopf. (8 h)

Enantioselective alkylation allylation and crotylation reactions (2 h)

Asymmetric oxidation [epoxidation (Sharpless, Jacobsen, Shi), dihydroxylation (Sharpless)], reduction (Noyori, Corey, Pfaltz)
(3 h)

Organocatalyzed asymmetric synthesis (2 h)

Desymmetrization, Kinetic resolution reactions (3 h)

Application of the above methods in synthesis of selected biologically relevant molecules. (5 h)

Suggested reading:

1. M. Nogrady, *Stereoselective Synthesis: A Practical Approach*, Wiley, 2008.

2. E. M. Carreira, L. Kvaerno *Classics in Stereoselective Synthesis*, Wiley-VCH: Weinheim, Germany, 2009.

3. K. C. Nicolaou, E. J. Sorenson, *Classics in Total Synthesis*, Wiley-VCH.

4. K. C. Nicolaou, S. A. Snyder, *Classics in Total Synthesis II*, Wiley-VCH.

Course Code : CY-574
Title of the Course : Advanced Magnetic Resonance

L-T-P : L / ~~T / P~~
Credits : 2 – 0 – 0

Prerequisite Course / Knowledge (If any): A course on Quantum Mechanics

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to

CLO-1: understand the magnetic resonance phenomenon

CLO-2 : understand how multidimensional, multinuclear NMR work
CLO-3: design new (multidimensional) NMR experiments based on theoretical calculations

CLO-4 : cope up with the requirements for higher-level research on NMR spectroscopy

CLO-5 : seek a job as technician/operator in NMR labs

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	2	2	1	2	2
CLO-2	3	3	3	3	3	2	2	3
CLO-3	3	3	3	2	3	1	1	3
CLO-4	3	3	3	3	2	2	1	3
CLO-5	3	3	3	2	2	1	2	2

Detailed Syllabus (CY-574)

Review of electron and nuclear spins - angular momentum and magnetic moment: classical and quantum descriptions

Larmor precession, energy levels, and Bloch equation

Angular momentum operators of single and coupled spins: density matrix, unitary transformation, spin angular momentum product operators, spin Hamiltonians, transformations under the influence of rf and microwave pulses, coherence transfer

Spin Relaxation

Scalar and Dipolar interactions, Fermi contact and hyperfine interactions

Chemical shift, g-value, anisotropy

Effect of distortion of structure and symmetry on g-value

Molecular structure determination from J-coupling and NOE constraints

Magnetic field gradients, molecular diffusion, NMR and EPR imaging

Suggested reading :

R R Ernst, G Bodenhausen, A Wokaun "Principles of Nuclear Magnetic Resonance in One and Two Dimensions" (Oxford Science)

Course Code : CY-576
Title of the Course : Computational Chemistry

L-T-P : L / ~~T/ P~~
Credits : 2 – 0 – 0

Prerequisite Course / Knowledge (If any): CY-403, CY-404, CY-453, CY-454, CY-503

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : understand bulk chemical processes at a molecular level

CLO-2 : develop concept of potential energy surfaces and understand their implications on reaction mechanism

CLO-3 : understand the celebrated Arrhenius equation and to learn derive it based on molecular level processes

CLO-4 : appreciate theories of reaction dynamics and their connection to the bulk chemical kinetics

CLO-5 : understand the transition state and its real time probing using femtosecond laser

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	3	1	2	1	3
CLO-2	2	3	2	2	1	2	1	3
CLO-3	3	2	2	3	1	2	1	3
CLO-4	2	3	2	2	1	2	2	3
CLO-5	3	3	2	3	1	2	2	3

Detailed Syllabus (CY-576)

Gas Phase Dynamics: Molecular beam scattering, Review of potential energy surface.
Dynamics of Molecular Collisions: Quasi-classical and quantum dynamics, cross section and rate constant. Microscopic mechanism of selected chemical reactions. Roming atom mechanism.
Microscopic interpretation of Arrhenius parameters.
Introduction to condensed phase dynamics, Krammer's theory and solvent effects.
Microscopic reversibility and detailed balance.
Marcus theory of electron transfer.
Femtochemistry- spectroscopic probing of transition state and control of chemical reactivity.

Suggested reading:

1. Theories of Molecular Reaction Dynamics, N. E. Henriksen and F. Y. Hansen, Oxford University Press.

2. Molecular Reaction Dynamics, R. D. Levine, Cambridge University Press.

3. Molecular Reaction Dynamics and Chemical Reactivity, R. D. Levine and R. B. Bernstein, Oxford University Press.

4. Tutorials in Molecular Reaction Dynamics, Eds. M. Brouard and C. Vallance, RSC Publishing.

Course Code : CY-577
Title of the Course : Computational Chemistry

L-T-P : L /Ŧ/ P
Credits : 1 – 0 –1

Prerequisite Course / Knowledge (If any): CY403, CY504

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : appreciate fundamental understanding of structure and bonding in chemistry on a practical perspectives

CLO-2 : appreciate that the theory of molecular quantum chemistry aid in deriving quantitative information on structure and properties

CLO-3 : learn practical tools to solve Hartree-Fock Equation and density functional theory equation

CLO-4 : learn improvement of basic method with various electron correlation methods

CLO-5 : carry out hand-on exercise to do quantum chemistry calculations with the state-of-the-art software

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	3	1	2	1	3
CLO-2	3	3	3	2	1	2	2	3
CLO-3	3	2	2	3	1	2	1	3
CLO-4	3	3	2	2	1	2	1	3
CLO-5	3	3	2	3	1	2	1	3

Detailed Syllabus (CY-577)

One hour lecture + two hours laboratory per week

Review of Electronic Structure Theory: Hartree-Fock, MP2, DFT and configuration interaction. Basis sets, convergence.

Geometry optimization, frequency calculation, location of transition state, intrinsic reaction coordinates, population analysis, natural bond orbital analysis, calculation of thermodynamic parameters.

Calculation of molecular excited electronic states.

Representative examples.

Suggested reading:

1. Quantum Chemistry, I. N. Levine, PHI Learning Private Limited.

2. Essentials of Computational Chemistry- Theories and Models, C. J. Cramer, John Wiley and Sons, Ltd.

3. Introduction to Computational Chemistry, F. Jensen, John Wiley and Sons, Ltd.

4. Computational Chemistry- a Practical Guide for Applying Techniques to Real-World Problems, D. C. Young, John Wiley and Sons, Ltd.

Course Code : CY579
Title of the Course : Elementary Polymer Chemistry

L-T-P : L ~~/ T / P~~
Credits : 2 – 0 – 0

Prerequisite Course / Knowledge (If any): MSc courses in the I - III semesters

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : understand the macromolecules, polymerization

CLO-2 : provide insight into the various classes of polymers and their synthetic process

CLO-3 : understand and analyze polymer molecular weights and various physical properties

CLO-4 : apply the basic concept of polymers in designing useful polymer materials

CLO-5 : apply the polymers for advanced applications.

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	2	2	1	1	3
CLO-2	3	3	3	2	2	1	1	2
CLO-3	3	3	3	2	3	1	1	2
CLO-4	3	3	3	3	2	3	2	3
CLO-5	3	3	3	3	3	3	2	3

Detailed Syllabus (CY-579)

Definition: Polymer, monomer, repeat unit, polymerization- Classification: Polymers based on source and polymerizations-polymer composition and structure- Nomenclature- IUPAC, Non-IUPAC, structure-based, and trade names- Types of polymers based on their molecular structure (linear, branched, cross-linked, block) and stereochemistry of repeating units (Tacticity in polymers)- Effect of Polymer structure on their properties (3 h)

Polymer Synthesis: Step, chain and miscellaneous polymerizations- Kinetics of polymerization- Anionic, Cationic, ATRP, ROMP, RAFT, Free radical polymerization- Polymerization of cyclic organic compounds - Reactions of synthetic polymers - Biological polymers - Inorganic elements in polymers- State of Polymerization: Emulsion, Dispersion, Solution, Solid-state etc. (6 h)

Polymer characterization - Chemical analysis of polymers, spectroscopic methods-IR, NMR, ESR, X-Ray Diffraction analysis- Microscopy- light Microscopy, Electron Microscopy and Electron Diffraction, Scanning electron microscopy- Thermal analysis- DSC, TGA, DMA, Rheology, Physical testing; stress-strain properties in tension (4.5 h)

Molecular Weights and Sizes: Solubility parameters, Thermodynamics of mixing, Flory-Huggins Theory for polymer solution, Flory-Huggins parameter, Polymer shape and size, measurement techniques-viscosity, colligative properties, chromatography, light scattering (Zimm plot) (3 h)

Physical State and Morphology: Crystalline and Amorphous state- Thermal transitions- Glass-Rubber transition - Mechanical properties– stress-strain behaviour - Elastomer, Fibers and Plastics (3 h)

Polymer Blend and Nanocomposites: Preparation, Types of blends, types of nanofillers, Thermodynamical considerations, Property enhancements, Uses (1.5 h)

Application of Synthetic Polymers: Materials and Biological importance and uses. Nanomaterials, Conducting polymers, Polymers for Energy applications. Physical aspects of polymers (1.5 h)

Suggested reading:

1. L. H. Sperling, Introduction to Physical Polymer Science, Wiley (1986)
2. H.R. Allcock and F.W. Lampe, Contemporary Polymer Chemistry, Prentice Hall (1990)
3. George Odian, Principles of Polymerization, 4th Edn, John Wiley (2004)
4. M. P. Stevens, Polymer Chemistry: An Introduction (2nd Edn), Oxford University Press (1990)
5. F.W. Billmeyer, Jr., Textbook of Polymer Science (1984), paperback
6. Relevant topics from modern literature

Course Code : CY-580
Title of the Course : Natural Products and Medicinal Chemistry

L-T-P : L / ~~T / P~~
Credits : 2 – 0 – 0

Prerequisite Course / Knowledge (If any): MSc courses in the I – III semesters

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : provide insight into natural products and medicinal chemistry

CLO-2 : appreciate the basic concepts related to natural products and medicinal chemistry

CLO-3 : apply the basic concepts of new natural products and medicinal compounds based on a fundamental understanding

CLO-4 : understand the synthesis of natural products and medicinal compounds

CLO-5 : apply different synthetic techniques for synthesis of natural products and medicinal compounds

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	2	2	2	1	3
CLO-2	3	3	3	2	2	2	2	3
CLO-3	3	3	3	2	2	2	1	3
CLO-4	3	3	3	3	3	3	2	3
CLO-5	3	3	3	2	3	3	2	3

Detailed Syllabus (CY-580)

Biosynthesis, total synthesis, structure elucidation and biological significance of selected natural products. (12 h)

Introduction to drug discovery: Sources of drugs-natural products, drugs from organic synthesis, drug discovery and development
(2 h)

Drug structure and biological activity-pharmaceutically important functional groups physicochemical properties of drugs, electronic effects, spatial properties of drugs Fate of drugs in the body-absorption, distribution, metabolism, and excretion. Chemistry of drug metabolism, modifications to decrease metabolism, prodrugs Molecular mechanism of drug action-drug targets, receptors, enzymes, nucleic acids, non-receptor targets
(5 h)

Chemistry of selected drug classes-pharmacodynamic, chemotherapeutic, antibacterial, antiviral, antineoplastic, cardio-vascular, CNS, antihistamine, diabetic, analgesic and antiinflammatory drugs.
(5 h)

Suggested reading:

1. K. C. Nicolaou, Classics in Total Synthesis, Vol 1, 2 and 3.
2. J. H. Fuhrhop, G. Li, Organic Synthesis: Concepts and Methods, 3rd edition, VCH, 1994.
3. J. Mann, Chemical Aspects of Biosynthesis, Oxford University Press, 1994.
4. R. B. Silverman, The Organic Chemistry of Drug Design and Action, 2nd edition, Elsevier, New York, 2004.
5. G. L. Patrick, An Introduction to Medicinal Chemistry-5, Oxford University Press, 2013.

Course Code : CY581
Title of the Course : Introduction to High Energy Materials

L-T-P : L / ~~T / P~~
Credits : 2 – 0 – 0

Prerequisite Course / Knowledge (If any): A course on undergraduate level physical and organic chemistry

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1 : understand the basic concepts related to the High Energy Materials (HEM)

CLO-2 : provide insight into the distinct characteristics of HEM

CLO-3 : understand and analyze the structure-property correlations in HEM

CLO-4 : characterization of HEM

CLO-5 : designing and applications of HEM

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8
CLO-1	3	3	3	2	2	2	1	1
CLO-2	2	3	3	3	3	2	2	1
CLO-3	1	2	3	3	3	3	2	2
CLO-4	1	1	1	2	3	3	3	2
CLO-5	1	1	1	2	3	3	3	3

Detailed Syllabus (CY-581)

Brief review of thermodynamics **[3 h]**
Laws of thermodynamics, Definition of heat, energy, internal energy, enthalpy, free energy and entropy. Relationship between ΔE and ΔH, Cp and Cv. Bond energy.

Thermo chemistry **[2 h]**
Standard enthalpy of formation, enthalpy changes in reactions, thermo chemical equations, heat of combustion, Hess Law, calculations of enthalpies for various types of reactions.

Requirement for High Energy Materials (HEM) **[5 h]**
Explanation for energy release using bond energy calculations, energy release with respect to heats of formation, heat of explosion, Density factor, oxygen balance.

Power of HEM **[2 h]**
Volume of gas and heat releases in an explosion, Pressure and temperature rise in an explosion reaction, explosive power and power index.

Decomposition reactions **[4 h]**
Decomposition products from explosion reactions: Kistiakowesky-Wilkinson rule, modified K-W rule, Springer-Robert rule, water-gas equilibrium, determination of composition of decomposition products using equilibrium chemistry.

Characterization of HEM **[4 h]**
Bomb calorimeter, Use of TG-DTA and DSC for determination of various energetic parameters of HEM.

Classification of HEM **[3 h]**
Classification based on chemical groups present, Activation energy required for initiation of HEM, Classification based on explosive power and energy required for initiation of HEM.

Burning of HEM **[2 h]**
Combustion, detonation and deflagration processes; propellants, explosives and pyrotechnics. Propellant and explosive compositions, fuel, oxidizers, binders, plasticizers, thermite mixture, and other ingredients.

Designing of HEM **[3 h]**
Synthesis of representative examples of HEM. Research directions, Specific applications of HEM

Reading materials:

1. Book: The Chemistry of Explosives, ISBN 0-85404-640-2, RSC Paperbacks 2004, Jacqueline Akhavan.
2. Book: Demystifying Explosives: Concepts in High Energy Materials, ISBN 978-0-12-801576-6, Elsevier 2015. _S. Venugopalan , HEMRL, Pune, India
3. Book: Introduction to Physics and Chemistry of Combustion: Explosion, Flame, Detonation, ISBN 3540787593, Springer 2008, Liberman Michael.

Course Code : CY-583
Title of the Course : C-H functionalization

L-T-P : L / ~~T / P~~
Credits : 2 – 0 – 0

Prerequisite Course / Knowledge (If any): CY-402, CY-452, CY-502

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students are expected to……

CLO-1: understand and learn the origin and multidirectional growth, concept/philosophy of C-H functionalization process in synthetic chemistry.

CLO-2: understand significant contributions of scientists who developed the concept of C-H functionalization processes in synthetic chemistry and the way in which they surmounted the problems/difficulties in the course of development of concept and philosophy of C-H functionalization processes.

CLO-3: understand and appreciate the importance and high level applicability of C-H functionalization process in synthetic chemistry for obtaining enantiomerically enriched /pure compounds as well as for synthesis of natural products and bioactive molecules.

CLO-4: understand, learn, and address the difficulties in the applications of C-H functionalization processes in advanced synthetic strategies.

CLO-5: have developed an interest in the subject and the ability to invent/design novel strategies for C-H functionalization processes that will be useful to industries.

Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

	PLO 1	**PLO 2**	**PLO 3**	**PLO 4**	**PLO 5**	**PLO 6**	**PLO 7**	**PLO 8**
CLO-1	3	3	3	3	3	3	3	3
CLO-2	3	3	3	3	3	3	3	3
CLO-3	3	3	3	3	3	3	2	**2**
CLO-4	3	3	3	2	3	3	2	**2**
CLO-5	3	3	3	2	3	3	2	2

Detailed Syllabus (CY-583)

1) Origin and earlier reports: Concept and classification of C-H functionalization, C-H functionalization of acidic C-H bonds, C-H functionalization of less acidic C-H bonds
2) Friedel-Crafts reaction, intramolecular Friedel-Crafts reaction, asymmetric intramolecular Friedel-Crafts reaction, application to synthesis of natural products and bioactive compounds
3) Free radical mediated C-H functionalization reactions, Breslow remote functionalization and applications, other reactions
4) Fujiwara–Moritani reaction, Heck reaction including asymmetric Heck reaction, intramolecular Heck reaction, asymmetric intramolecular Heck reaction, application to synthesis of natural products and bioactive compounds, Catellani reaction
5) Baylis-Hillman reaction, asymmetric Baylis-Hillman reaction, intramolecular Baylis-Hillman reaction, asymmetric intramolecular Baylis-Hillman reaction, application to synthesis of natural products and bioactive compounds
6) C-H functionalization *via* C-H activation, origin of C-H bond activation and earlier reports, development of concept of C-H functionalization *via* C-H activation, asymmetric C-H functionalization *via* C-H activation, intramolecular version, asymmetric intramolecular version, application to synthesis of natural products and bioactive compounds
7) Miscellaneous reactions

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