M.Sc. Curriculum

2017 - 2019

Department of Chemistry

National Institute of Technology Sikkim

Curriculum for 2 Year M.Sc. Programme

FOR ACADEMIC YEARS 2017 - 19

Semester	Subject Code	L-T-P	Subject Name	Credit
First	CY21101	3-1-0	Organic Chemistry – I	4
	CY21102	3-1-0	Inorganic Chemistry – I	4
	CY21103	3-1-0	Physical Chemistry – I	4
	CY21104	3-0-0	Biochemistry – I	3
	CY21105	2-1-0	Mathematics for Chemists	3
	CY21201	0-0-6	Organic Chemistry Laboratory – I	3
	CY21202	0-0-6	Inorganic Chemistry laboratory – I	3
			Total Credit	**24**

Semester	Subject Code	L-T-P	Subject Name	Credit
Second	CY22101	3-1-0	Organic Chemistry – II	4
	CY22102	3-1-0	Inorganic Chemistry – II	4
	CY22103	3-1-0	Physical Chemistry – I	4
	CY22104	3-1-0	Biochemistry – II	4
	CY22105	3-1-0	Spectroscopy - I	4
	CY22201	0-0-6	Organic Chemistry Laboratory – II	3
	CY22202	0-0-6	Inorganic Chemistry laboratory – II	3
			Total Credit	**26**

Semester	Subject Code	L-T-P	Subject Name	Credit
Third	CY23101	3-1-0	Organic Chemistry – III	4
	CY23102	3-1-0	Inorganic Chemistry – III	4
	CY23103	3-1-0	Physical Chemistry – III	4
	CY23104	3-1-0	Spectroscopy – II	4
	CY2330W	3-0-0	Elective - I	3
	CY23201	0-0-12	Physical Chemistry Laboratory & Computational Laboratory	6
	CY23202	0-0-8	Mini Project	4
			Total Credit	**29**

Semester	Subject Code	L-T-P	Subject Name	Credit
Fourth	CY2430X	3-0-0	Elective - II	3
	CY2430Y	3-0-0	Elective - III	3
	CY2430Z	3-0-0	Elective - IV	3
	CY24201	0-0-24	Major Project	12
			Total Credit	**21**
ALL			**Grand total Credit**	**100**

L: Lecture hour per week; **T**: tutorial hour per week; **P**: Practical hour per week.

Semester-I

CY21101: ORGANIC CHEMISTRY-I

L	T	P	C
3	1	0	4

Module 1 Basic Organic Mechanisms

Basic reaction mechanisms of aliphatic & aromatic electrophilic & nucleophilic reactions, reductions, oxidations, protective groups, Elimination reactions, concepts of diastereo- and enantioselectivity, uses of phase transfer catalysts, ultrasound, solid phase syntheses using polymer support, crown ethers.

Module 2 Stereochemistry - I

Newman, Sawhorse, Fisher projections, D,L- and R,S, Re-Si nomenclatures, Acyclic systems up to 4 chiral centres: compounds with asymmetric carbons in branched chains, point groups, correlation of axial dissymmetry and and centrodissymmetry, conformational analysis of cyclopropanes, cyclobutane, cyclopentane, cyclohexene, variously substituted cyclohxanes, decalins, Cram's rules, Felkin-Anh model, Prelog's rule.

Module 3 Photochemistry

Basic principles, Jablownski diagram, photochemistry of olefinic and carbonyl compounds, cis- / trans-photoisomerism, stereomutation, Norrish Type I and II reactions, Di-Pi-Methane (DPM), rearrangement, Aza-DPM, Paterno-Buchi reaction, photochemistry of arenes, photoreductions of ketones, method of generation and dection (ESR) of radicals, radical cyclisations, Baldwin's rules, substitution, addition and insertion reactions involving radicals, allylic halogenation, autooxidation, Barton reaction.

Module 4 Pericyclic Reactions

Classification and stereochemical modes, Thermal and Photo reactions, Selection rules, electrocyclic, cycloaddition, chelotropic, sigmatropic rearrangements, carbine addition, rationalization by FMO, Zimmerman, Mobius-Huckel methods, metal catalyzed cycloaddions., Ene reaction.

Module 5 Natural Products I

Familiarity with methods of structure elucidation (chemical & spectroscopic), synthesis, biosynthesis, biogenesis of representative examples of acyclic, monocyclic and bicyclic mono- / di-terpenes, like carvone, camphor, citral, pinenes, abietane, ebietic acid, Gutta-Percha, vulcanized rubber, etc.

CY21102: INORGANIC CHEMISTRY - I

L	T	P	C
3	1	0	4

Module 1 (Molecular Structure & Bonding)

LCAO-MO methods in homo and heteronuclear diatomic molecules, bonding in triatomic molecules, VSEPR theory, hybridization, Walsh diagram, Bent's rule, structure and reactivity of covalently bonded molecules Atomic and ionic radii–bond length, bond strength. Hydrogen bonding interactions, effect of hydrogen bonding and other chemical forces on melting, boiling and solubility.

Module 2 (Non-transition Metal Chemistry)

Synthesis, Properties, Structure and Bonding of: Nitrogen, Phosphorous, Sulfur, Pseudohalogen, Interhalogen and Xenon Compounds; Boranes, Carboranes, Metallocarboranes, Borazines, Phosphazenes, Sulfur-Nitrogen compounds, silicates, silicones. Iso- and Hetero-poly anions. Redox Reactions: Latimer diagram, Electrochemical Series. Acids and Bases: Lewis acids and bases; HSAB concept.

Module 3 (Metal Chemistry Chemistry-I)

Bonding in Coordination Complexes: Crystal-Field theory, d-orbital Splitting in Octahedral, Tetrahedral, Square Planar geometries; Molecular Orbital Theory, p-bonding; Jahn-Teller effect, Spectrochemical series, nephelauxetic series. Electronic Spectra: Selection Rules, d-d transitions, charge-transfer spectra.

Module 4 (Symmetry & Group Theory)

Group Theory: Definition of group, symmetry, point groups, representation of group, orthogonality theorem, irreducible representation, character table, direct sum, direct product, derivation of projection operator. Application of symmetry, the symmetries of molecular orbitals (symmetry-adapted linear combinations, construction of MOs, the vibrational analogy).

L	T	P	C
3	1	0	4

CY21103: PHYSICAL CHEMISTRY-I

Module 1 (Thermodynamics)

Brief review of 1st, 2nd and 3rd laws of thermodynamics, Nernst heat theorem and the third law of thermodynamics, calculation of entropy changes in chemical reactions. Mathematical and thermodynamic probability, Entropy and probability, the free energy of a mixture, Partial molal quantities, Analytical form of the chemical potential in ideal solutions, Chemical potential of a solute in a binary solution, Application of Gibbs-Duhem equation, Nonideal solutions, concept of activity: experimental determination of activity coefficients of non-electrolytes.

Module 2 (Quantum Chemistry-I)

Schrödinger equation, Basic postulates and theorems, Physical interpretation of wave function, stationary states, operator formation, atomic unit system, Heisenberg's equation of motion, Particle in a box problem, Finite barrier problem and tunneling, Linear harmonic oscillator, Ladder operators, Angular momentum problem, Rigid rotor, Hydrogen atom problem and its implications.

Module 3 (Chemical Kinetics I)

Composite Reactions – types of composite mechanisms, rate equations for composite mechanisms, simultaneous and consecutive reactions, steady state treatment, rate determining steps, microscopic reversibility and detailed balance, chain reactions (H_2-Br_2 reaction, decomposition of ethane and acetaldehyde) and oscillatory reactions (BelousovZhabotinskii reaction).

Module 4 (Micelles and Colloids)

Surface active agents and their classification, micellization, hydrophobic interaction, critical micellar concentration (cmc), factors affecting cmc of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsions, reverse micelles. Multimolecular, macromolecular and associated colloids. Stability of colloids. The zeta potential. Kinetic, optical and electrical properties of colloids. Electrokinetic phenomena: Electrophoresis, electroosmosis, sedimentation potential and streaming potential. Donnan

membrane equilibrium. Collodal quntum dots, Metal nanoparticles and magnetic nanoparticles. Size dependent optical and electrical properties. Supermagnetic limit.

CY21104 BIOCHEMISTRY (same as BT13103 of Biotechnology BTech 3rd Semester)

L	T	P	C
3	1	0	3

Module 1 (16 hours**)**

Glycolysis, TCA cycle, Glyoxylate cycle, Gluconeogenesis, β-Oxidation of fatty acids, Omega oxidation, Ketone bodies, Biosynthesis and degradation of amino acids, Regulation and disorders of amino acid metabolism, Biosynthesis of fatty acids, Eicosanoids, Triglycerols, Degradation of cholesterol and steroids, Photosynthesis-photosystem I and photosystem II,

Module 2 (09 hours)

Biosynthesis and catabolism of purines and pyrimidine, Preliminery idea of De novo synthesis and Salvage pathway, Regulation and disease due to defect in nucleotide metabolism

Module 3 (11 hours)

Oxidative phosphorylation, Role of membrane-bound carriers in electron transfer, Synthesis of ATP, Regulation of oxidative phosphorylation, Uncouplers, Biological transport, structure and properties of biological membranes, passive transport and active transport, glucose, Na^+ and K^+ transport.

Module 4 (10 hours)

Introduction to structure of deoxyribonucleic and ribonucleic acid, Base pairing, Base stacking, Stabilized forms of DNA-A, B and Z forms, Melting of DNA double helix

References:

1. D. L. Nelson and M. M. Cox, Lehninger Principles of Biochemistry, 4th Edn, WH Freeman and Company, 2005.
2. J.M. Berg, J.L. Tymoczko, and L. Stryer, Biochemistry, 6th Edn., WH Freeman and Company, 2007.
3. R. H. Garret and C. M. Grisham, Biochemistry, 3rd Edn., Brooks Cole, 2004.
4. D. Voet and J.G. Voet, Biochemistry, 3rd Edn., John Wiley & Sons Inc., 2004.
5. G.L. Zubey, Biochemistry, 4th Edn,Wm. C. Brown Publications, 1998.
6. W. H. Elliot and D.C. Elliot, Biochemistry and Molecular Biology, 4th Edn, Oxford University Press, USA, 2009.

CY21105: MATHEMATICS FOR CHEMISTS

L	T	P	C
3	1	0	3

Module 1

Functions Differential and integral calculus, limits, derivative, physical significance, basic rules of differentiation, maxima and minima, applications in chemistry, exact and inexact differential, periodic function, Taylor and McLaurin series, curve sketching, partial differentiation, rules of integration, definite and indefinite integrals.

Module 2

Differential equations Separation of variables, homogeneous, exact, linear equations, equations of second order, series solution method. Fourier series and analysis. Complex numbers. Laplace transformation.

Module 3

Permutations, combinations and theory of probability Distributions. Vectors, matrices and determinants: Vectors, dot, cross and triple products, introduction to matrix algebra, addition and multiplication of matrices, inverse, adjoint and transpose of matrices, unit and diagonal matrices. Complex Variables.

Module 4

Numerical Methods Roots of Polynomials, Solution of Linear simultaneous equations, matrix multiplication and inversion. Numerical integration. Statistical treatment of data, variance and correlations, Least square curve fitting. Computer programming in FORTRAN. Computer application in Chemistry: Development of small computer codes involving formulae in chemistry. Evaluation of lattice energy and ionic radii from experimental data, Linear simultaneous equations to solve secular equations within the Huckel theory.

L	T	P	C
0	0	6	3

CY21201: Organic Chemistry laboratory – I

Quantitative Analysis: Determination of the percentage/ number of hydroxyl groups in an organic compound by acetylation method. Estimation of amines / phenols using bromate – bromide solution/ acetylation method. Determination of iodine and sponification values of an oil sample. Determination of DO, COD and BOD of water sample.

Single step reactions like nitration of aromatics; reduction of nitro to amine; protection of alcohol, amine; LAH, $NaBH_4$ reductions of ester / ketone / aldehydes; Diels-Alder reaction with Anthracene and Maleic anhydride; etc.

CY21202: Inorganic Chemistry laboratory – I

L	T	P	C
0	0	6	3

1. Qualitative analysis of radicals in a given mixture comprising of less common metals (Be, Mo, W, Ti, Zr, Th, V, U, Cr and all the radicals included in B.Sc. (Honours) Chemistry syllabus.
2. Simple experiments will be conducted to elucidate the working principles, instrumentation and handling of Gas Chromatograph, UV-Vis spectrometer, IR spectrometer, Oxygraph (Measurement of gaseous oxygen by Clark type electrode), conductivity meter, pH meter and Nephlometer

Essential Reading

1. G. Svehla, *Vogel's qualitative inorganic analysis*, Harlow Longman, 2002.
2. A I Vogel, John Bassett, *Vogel's textbook of quantitative inorganic analysis: including elementary instrumental analysis*, Longman, 2003.
3. R.C. Das and B. Behera, *Experimental Physical Chemistry, ,* Tata McGraw Hill 2000.

Semester-II

L	T	P	C
3	1	0	4

CY22101: ORGANIC CHEMISTRY-II

Module I: Reagents in Organic synthesis

Use of the reagents in organic synthesis and functional transformations, Organometallic reagents, Metal hydride, Gilman's reagent, LiCuMe2, LDA, DCC, 1,3-dithane, Oxidizing and reducing agents, Peterson's synthesis, Laweson's reagent, Wilkinson's catalyst, baker Yeast, hypervalent organo Iodines. Reagents of transition and non-transition metals-Zn, Cd. Chemistry of organo sulphur, organo phosphorus and organo Silicon compounds, organoboron compounds.

Module II: Rearrangement Reaction/ Selective organic reaction/Name reactions

Heck, Stille, Suzuki Coupling, Sonogashia, Buchwald-Hartwig, Ziegler Natta reaction, Olefin metathesis, Carbene generation, Birch Reduction, Cannizaro, Condensation reaction (Aldol, Benzoin), Formation and reaction of Carbene, Rearrangement reaction, Sharpless asymmetric epoxidation, Advanced name reactions.

Module III: Synthetic Strategy

Retrosynthtic Analysis, Disconnection approach, Functional group Disconnection approach, Functional group interconversion, Umpoulung (1, 3-dithane), convergent Synthesis, Design of multistep synthesis.

Module IV: Basic of heterocyclic compounds

Aromaticity of heterocyclic compounds, Synthesis of Heterocyclic ring containing oxygen, nitrogen, Sulphur and reactions.

Module V: Natural Products II

Occurrence and role of chemical ingredients in nature, Synthesis of naturally occurring compounds, Stereochemistry of naturally occurring compound, chirotopial properties of organic molecule, CD, ORDVCD principles and application, Allenes, Biphenyl system.

CY22102: INORGANIC CHEMISTRY-II

L	T	P	C
3	1	0	4

Module 1 (Organometallic Chemistry-I)

18-electron rule, metal carbonyls, nitrosyls, cabonyl hydrides, isolobal analogy, dioxygen and dinitrogen compounds. Metal alkyls, carbenes, carbynes, alkenes, alkynes, and allyl complexes. Hydrides, Metallocenes, Metal arene complexes. Carbonylate anions, agostic interaction, Oxidative addition and reductive elimination, insertion and elimination reactions. Homogeneous and heterogeneous catalysis. Fluxional molecules. Metal-Metal bonding and Metal clusters.

Module 2 (Reaction mechanism of transition metal complexes)

Substitution reactions in square planar complexes, Trans effect, mechanism of the substitution reactions, nucleophilicity parameters, *etc*.

Redox reactions-complementary and non-complementary reactions, mechanisms of outer sphere and inner sphere electron transfer reactions, theory of outer sphere processes, the Marcus cross relation.

Module 3 (Transition Metal Chemistry-II)

Magnetic properties, paramagnetism, ferro- and antiferro magnetism, diamagnetism, Pascal constants, Curie equation, Russell-sander's terms, determination of magnetic susceptibility, magnetic properties of first transition series metal ions and lanthanides. CFT and its limitations, Orgel and Tanabe-Sugano diagrams and spectra, calculations of Dq, B and b-parameters, charge transfer spectra, anomalous magnetic moment, magnetic exchange coupling and spin crossover.

Module 4 (Lanthanides & Actinides)

General discussion on the properties of the f-block elements. Spectral and Magnetic properties,. Photochemistry & Photophysics of Lanthanide compounds. Application of lanthanide & actinide compounds (as shift reagents, chemosensors, applications in cancer diagnosis & therapy, etc.).

CY2213: PHYSICAL CHEMISTRY-II

L	T	P	C
3	1	0	4

Module 1 (Statistical Thermodyanmics)

Concept of distribution, thermodynamic probability and most probable distribution, Ensemble averaging, postulates of ensemble averaging, Canonical, grand canonical and micro canonical ensembles, corresponding distribution laws (using Lagrange's method of undermined multipliers). Partition functions-translational, rotational vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions. Applications of partition functions, Heat capacity behaviour of solids-chemical equilibria and equilibrium constant in terms of partition functions.

Module 2 (Quantum Chemistry II and Group Theoretical Techniques)

The variational method, Eckart's theorem, Linear variational method, Perturbation theory (time independent), Application of variational method and nondegenerate perturbation theory to the helium atom problem. Electron spin, Antisymmetry principle, Degenerate perturbation theory and its application to Zeeman and anomalous Zeeman effect, Stark effect. Huckel M.O. theory for conjugated systems, bond order and charge density calculations, Introduction to the method of self consistent Field, Hartree method, Koopman's theorem.

Time dependent perturbation theory: Harmonic perturbation and Fermi golden rule, Einstein's coefficients of induced emission and absorption. Reducible and irreducible representations, classes and characters, Great Orthogonality and related theorems, Projection operator, Direct product representation Applications: SALC, Spectroscopic selection rules, Polyatomic vibration and normal modes.

Module 3 (Polymers)

Polymers-definition, types of polymers, Molecular mass-number and mass average molecular mass, determination of molecular mass (osmometry, viscosity, light scattering meth0ods, Gel Permeation chromatography). Plastics, elastomers and fibers, kinetics of polymerization

Module 4 (Bio-Physical Chemistry)

A. Interactions in Biological Systems

Intra and inter molecular forces, electrostatic interactions and Hydrogen bonding interactions, van der Waals and Hydrophobic interactions, Disulphide bridges, Role of water and weak interactions.

B. Spectroscopic techniques for bio-physical chemistry

UV, visible and Fluorescence spectroscopy, X-ray Diffraction, Nuclear Magnetic Resonance (NMR), Mass Spectrometry

CY22105: Biochemistry - II

L	T	P	C
3	1	0	4

Module 1 Supramolecular Chemistry

From molecular to supramolecular chemistry, factors leading to strong binding (non-covalent interactions), new molecular receptors, crown ethers, siderophores, cyclophanes, cyclodextrin and their applications in specific recoginitions, supramolecular reactivity and catalysis, switching devices, self-assembly of aggregates, crystal engineering, importance of molecular recognitions in life processes.

Module 2 Bioorganic Chemistry

Molecular models of biological receptors, biomimetic chemistry, design synthesis and binding studies of synthetic receptors, Enzyme models, micelles, biopolymers, catalytic antibodies, principle of gene synthesis, gene delivery, gene therapy, antisense therapy.

Module 3 Bioinorganic Chemistry-I

Role of alkali and alkaline earth metal ions in biology; Na^+ -K^+-Pump, ionophores and crown ethers. Metal site structure, function. Metal ion transport and storage: Ferritin, Transferrin, Siderophores and metallothionein. Electron Transfer: Cytochromes, Iron-Sulfur Proteins and Copper Proteins.

Module 3 Bioinorganic Chemistry-II

Oxygen transport and storage: Hemoglobin, myoglobin, hemerythrin, hemocyanin Oxygen activation: Cytochrome P450, Cytochrome c oxidase. Other metal containing enzymes: Catalase, peroxidase, superoxide dismutase, alcohol dehydrogenase, carbonic anhydrase, carboxypeptidase, xanthine oxidase, nitrogenase, vitamin B12 coenzyme, photosystem I and II, oxygen evolving center.

CY22105: Spectroscopy-I

L	T	P	C
3	1	0	4

Module 1

Light absorption and emission, shape and intensity of absorption and emission bands. Franck-Condon principle, Kasha's rule, photophysics of radiative and non-radiative transitions, energy transfer processes, Excimers and exciplexes, Fluorescence and phosphorescence, Quantum yield, life time and anisotropy, static and dynamic quenching, Stern-Volmer analysis.

The Electromagnetic radiation, Absorption and emission spectra, Effect of radiation on atoms and molecules, Subdivisions of spectroscopy. Basic principles of Vibrational, Rotational and electronic Spectroscopy: Linear oscillator, rotor model, selection rules, Rayleigh scattering. Vibrating diatomic molecules, interaction of vibration and rotation, vibrations of polyatomic molecules, impact of rotation on polyatomic molecules.

Module 2

Electronic spectra of diatomic molecules, vibrational coarse structure, progressions, intensity of vibrational-electronic spectra: the Franck-Condon Principle, oscillator strengths, spectroscopic and equilibrium dissociation energies, Molecular term symbol, $n \rightarrow \pi$, $\pi \rightarrow \pi$ transition.

Module 3

Principle of Microwave spectroscopy: Rotation of molecules, rotational spectra, diatomic and polyatomic molecules, instrumentation, chemical analysis by microwave spectroscopy. Raman Spectroscopy: Polarization of light and the Raman Effect, pure rotational Raman and vibrational Raman spectra, structure determination from combined Raman and IR spectroscopy. Rotational fine structure of electronic-vibration transitions.

Module 4

Steady state Fluorescence: Principles**,** Jablonski diagram, application of fluorescene spectroscopy, Basic instrumentation, Effect of solvents on fluorescence spectra (general and specific), Chemical and biochemical applications of anisotropy measurements. Flash photolysis, laser flash photolysis.

CY22201: Organic Chemistry laboratory – II

L	T	P	C
0	0	6	3

Multistep Synthesis: Cannizzaro reaction: 4-chlorobenzaldehyde as substrate. Benzilic Acid Rearrangement:

Benzaldehyde → Benzoin → Benzil → Benzilic acid.

Hofmann bromamide Rearrangement: Phthalic anhydride-Phthalimide → Anthranilic acid

Beckmann Rearrangement: Benzene → Benzophenone → Benzophenone oxime → Benzanilide.

Skraup Synthesis: Preparation of quinoline from aniline.

Synthesis using Phase Transfer Catalysis: Alkylation of diethyl malonate or ethyl acetoacetate and an alkyl halide.

Peckmann Condensation for Coumarin

Three-component synthesis: Dihydropyrimidinone

CH 2221: Inorganic Chemistry laboratory – II

L	T	P	C
0	0	6	3

Preparation of Inorganic compounds/complexes and their physico-chemical characterization by different spectroscopic (IR, UV-Visible, NMR *etc*.) & magnetic susceptibility measurements. Depending on the availability of reagents/instruments compounds/complexes will be selected from the list given below:

(i) Transition metal acetylacetonates

(ii) *Cis*- and *trans*-dichlorobis(ethylenediamine)cobalt(III) chloride

(iii) *Tris*(ethylenediamine)cobalt(III) chloride

(iv) Nitropentaminocobalt(III) chloride

(v) *Cis*- and *trans*-bis(glycinato)copper(II)

(vi) Ru(II/III) complexes of bipy

(vii) Sodium tetrathionate

Essential Reading:

1. In-house laboratory manual and relevant literature

2. G. Svehla, *Vogel's qualitative inorganic analysis*, Harlow Longman, 2002.

3. A. I. Vogel, John Bassett, *Vogel's textbook of quantitative inorganic analysis: including elementary instrumental analysis*, Longman, 2003.

Supplementary Reading:

5. A. I. Vogel, *Qualitative Inorganic Analysis*, Orient Longman – 1979.

Semester-III

CY23101: ORGANIC CHEMISTRY-III

L	T	P	C
3	1	0	4

Module 1 Advanced Heterocyclic Chemistry

Indoles, pyrimidines, pyrazidines, pyrazines, purines, pteridines, biosynthesis of nucleotides, Role of heterocycles in biological systems.

Module 2 Medicinal Chemistry

Antibiotics – Penicilins, tetracyclins, analgesics, prostaglandins synthesis, role of enzymes, Drug-receptor interactions, mechanism of drug actions, agonists, antagonists, phrmacokintecis: drug absorption, distribution, metabolism, excretion, examples of drug design, synthesis, molecular modeling.

Module 3 Carbohydrate Chemistry

Basic structure and type of sugars, Protection / deprotection strategies, orthogonality, glycosylation methods, armed-disarmed concept, glycals, deoxy-sugars, aminosugars, cyclitols, polysaccharide synthesis, polysaccharides as vaccines, importance of carbohydrates as chiral pool.

Module 4 Natural Products II

Familiarity with methods of structure elucidation (chemical & spectroscopic) biosynthesis and biological activity of alkaloids – nicotine, atropine, conine, papaverine, cinchona group, isoquinoline alkaloids – morphine, ephedrine, thibein; Steroids: occurrence, nomenclature, basic skeleton, synthesis and stereochemistry, biosynthesis of flavonoids, lignans.

Module 5 Asymmetric Synthesis

Enzymatic and catalytic asymmetric induction, reactions of enolates, use cinchona alkaloid derivatives, cross aldol, chiral metal complexes for cyclopropanation, epoxidation, AD-mix, Ender’s catalyst, Corey catalyst,

CY23102: INORGANIC CHEMISTRY-III

L	T	P	C
3	1	0	4

Module 1 (Spectroscopic Techniques in Inorganic Chemistry)

Various spectroscopic methods used in Inorganic chemistry: X-ray diffraction, electronic spectra, EPR (emphasis on first row transition metal ions and their spectra), brief description of CD / MCD and multinuclear NMR. Applications of newer methods like EXAFS, XANES and ENDOR in characterization of biological molecules.

Module 2 (Organometallic Chemistry-II)

Definition, classifications and bonding in organometallic compounds. Isolobal analogies. Structural methods of Organometallics. Preparative methods. Spectroscopic techniques in organometallic chemistry. Electronic and magnetic properties of Organometallic compounds. Stoichiometric and catalytic reactions. Fundamental processes in reactions of organo-transition metal complexes. Applications of transition metal complexes to catalysis, organometallics directed towards organic synthesis. Bio-organometallics, Organometallics in environmental chemistry. Metal clusters and models for heterogeneous catalysis. Application of Organometallics in Industry.

Module 3 (Introduction to Solid-state & Materials Chemistry)

Synthesis of materials, Defects and ion transport, Metal oxides, nitrides & fluorides, Chalcogenides, Intercalation compounds & metal-rich phases, Framework structures, Hydrides & hydrogen-storage materials, Semiconductor Chemistry, Molecular materials (Single molecular magnets, 1-D metals, Liquid crystals).

Module 4 (Chemical Toxicity and metallotherapy)

Toxic chemicals in the environment; toxic effects of arsenic, cadmium, lead, mercury, carbon monoxide, cyanide and other carcinogens; metal containing drugs in therapy; interaction of heavy metal ions with DNA; DNA cleavage; structure-activity relationship and mode of action

CY23103: PHYSICAL CHEMISTRY-III

L	T	P	C
3	1	0	4

Module 1 (Electrochemistry)

Theory of electrolytes, Ion-electron theory; Debye Huckel Limiting law, Activity Coefficients, Theory of electrified interfaces, Guoy-Chapman, Stern, Tobin etc. models; overpotential, exchange current density, bulter volmer equation, Tafel plot. Polarizable and non-polarizable interfaces. Electrochemical cells and Batteries.

Quantum aspect of charge transfer at the electrode – solution interfaces, Electrocapillarity (EC), nature of EC curves, Lipmann equation, Electrical double layer theory. Electrochemistry at semiconductor interfaces; Electrocatalysis, Photoelectrochemistry, Theory and application of polarography, cyclic-voltammetry.Bioelectrochemistry; Introduction to corrosion, forms of corrosion, corrosion monitoring and prevention methods.

Module 2 (Solid-State)

Bragg-Miller indices, X-ray structural analysis of crystals, identification of unit cells, structure of simple lattices and X-ray intensities, Defects in solids: point, line and plane defects, Determination of equilibrium concentration of Scottky and Frenkel defects, F-centres/color-centres in ionic crystals, Band theory of solids, Semiconductors (extrinsic and intrinsic), hopping semi-conductors, rectifiers, transitors, Super conductivity, Organic conducting solids, solid state reactions.

Module 3 (Non-equilibrium Thermodynamics)

Thermodynamic criteria for non-equilibrium process, Entropy production and entropy flow, Entropy balance equations for heat flow, chemical reactions etc., Transformations of the generalized fluxes and forces, Nonequilibrium stationary states, Generalized flux and forces, Phenomenological equations, Onsager reciprocal relations, Principle of detailed balance, Electro kinetic phenomenon, Diffusion, Electric conduction, Transport number and electrochemical cells, Irreversible thermodynamicc for biological systems.

Module 4 (Chemical Kinetics II)

Methods of determining rate laws, collision theory of reaction rates, Arrhenius equation and activated complex theory. Potential energy surfaces. Unimolecular reactions and their treatments (Lindemann-Hinshelwood, Rice-Ramsperger-Kassel [RRK], and Rice-Ramsperger-Kassel-Marcus [RRKM] theory). Experimental Methods: Enzyme kinetics, studies of fast reactions by flow method, relaxation method, flash photolysis and NMR.

CY23103: Spectroscopy -II

L	T	P	C
3	1	0	4

Module 1 NMR

Instrumentation and application of infrared spectroscopy for functional group determination; Instrumentation and applications of UV-Visible spectroscopy. Principle and application of NMR spectroscopy, Factors influencing chemical shifts, Spin-Spin interaction, coupling constant, Classification of ABX, AMX, ABC, A2B2 in proton NMR; ^{13}C NMR and DEPT NMR. structure determination of organic compounds using UV-Visible, Infrared and NMR spectra. Heteronuclear coupling, Pulse NMR spectroscopy and techniques, relaxation time and their importance, determination of relaxation times, Temperature dependent NMR and molecular dynamics, Elementary ideas on 2D NMR spectroscopy (^{1}H-^{1}HCOSY, NOESY, HMQC, HSQC, HMBC), Extension to other nuclei (^{19}F, ^{31}P etc). ***Structure elucidation of Organic Compounds***: Use of spectroscopic techniques for structure determination and other applications.

Module 2 Mass Spectrometry

Principle, Instrumentation, applications and Mass spectral techniques, EI, CI, FD, FAB and MALDI, Small molecule fragmentation patterns of organic compounds like McLafferty rearrangement; tandem MS/MS, protein structure analysis, microarray, concepts in bioinformatics.

Module 3

Photoelectron spectroscopy, EXAFS, The influence of nuclear spin and the Zeeman effect. Spin resonance Spectroscopy: Basic Concepts, Nuclear spin states, mechanism of absorption, population densities of nuclear spin states, NMR Spectrometer. Electron Paramagnetic Resonance: Underlying principle, presentation of spectra, instrumentation, hyperfine splitting (applications to radicals). **Mössbauer Spectroscopy:** Basic principles, spectral parameter Applications – oxidation states of iron compound. Mass spectral techniques

Module 4

X-ray diffraction: Basics of X-ray Diffraction. Crystal Growth: Crystallization techniques, Evaluation of crystals. Data Collection: Crystal selection, Operation of instrument, Data collection methods. Data Solving and Refining, X-ray structure determination, Direct methods, Patterson methods, Structure refinement Interpretation of results, Disorder and twinning, Publishing and Presenting Results, Crystallography tables and information files, Crystallographic database, Graphics

CY23201: Physical Chemistry Laboratory Computational Laboratory

L	T	P	C
0	0	12	6

Physical Chemistry (Perform any 5 experiments)

1. Studies on the kinetics of iodination of acetone.
1. Determination of coordination number of Cu^{++} (partition method).
2. Ion exchange capacity of resin.
3. Verification of Beer's law and studies on the kinetics of alkaline hydrolysis of crystal violet.
4. Estimation of acid potentiometrically.
5. Estimation of acid pH metrically.

7. Determination of pK_1 and pK_2 of phosphoric acid potentiometrically.
8. Studies on the kinetics of reaction between $K_2S_2O_8$ and KI spectrophotometrically.
9. Ternary phase diagram of $H_2O/C_6H_6/CH_2COOH$.
10. Determination of CMC and micellization parameters of an ionic surfactant conductometrically.
11. Determination of the activation energy of the reaction between $KBrO_3$ and KBr.
12. Estimation of Cl^-, Br^- and I^- in a mixture potentiometrically.
13. Determination of composition of Fe^{2+}- salicylate complex by Job's method.

Physical Chemistry and Computational Chemistry Lab (Perform any 5 experiments)

1. Determination of pK_a of methyl red indicator spectrophotometrically.
2. Determination of pK_a of phenolphthalein indicator spectrophotometrically.
3. Study the effect of ionic strength on the kinetics of $K_2S_2O_8$ + KI reaction.
4. Study on the effect of ionic strength on the kinetics of $KBrO_3$ + KBr reaction.
5. Study the kinetics of inversion of cane sugar polarimetrically.
6. Determination of electronic properties (molecular energies, orbitals etc.) of simple molecules e.g. (H_2O, C_6H_6) using Hatree-Fock, Density functional calculations.
7. Determination of structural features such as bond lengths, bond angles, dihedral anges of molecules extracted from Cambridge Crystallographic database.

Electives

Elective 1:

Pharmaceutical Chemistry

Module 1 Pharmacology

General Pharmacology: Introduction, Routes of Administration of Drugs, Mechanism of action of Drugs (Absorption, Distribution, Metabolism and Excretion of Drugs), Basic idea of mechanism of Drug action, Drug Toxicity, Pharmacology of ANS - Neurohumoral transmission, Drug acting on Sympathetic and Parasympathetic, Drugs acting on CNS - Sedative and Hypnotic agents, Hypoglycemic agents, Respiratory pharmacology: Drugs used in the treatment of various disorders of the respiratory tract, Antiviral drugs, Cancer chemotherapy,

Module 2 Pharmacokinetics

Principles of Pharmacokinetics: first order, zero order, Biological half life; Pharmacokinetics of Multiple; Dosing; Dosage regimen design based on mean average; minimum and maximum plasma concentrations; Concept of Steady state plasma concentration and Renal clearance; One compartmental open model and calculation; Basic idea of two compartmental model and its use, concept of AUC, Cmax , Tmax , Absorption and Elimination rate constants, lag time, onset of action, duration of action, termination of action, Flip-flop phenomena. Non-Linear Kinetics: Special reference to Michaelis-Menten equation.

Module 3 Medicinal Chemistry II

Physicochemical aspects (Optical, geometric and bioisosterism) of drug molecules and biological action, drug receptor interaction including transduction mechanisms.

ACTIVITY RELATIONSHIP INCLUDING PHYTOCHEMICAL PROPERTIES OF THE FOLLOWING CLASSES OF DRUGS:

A) Drugs acting at synaptic and neuroeffector junction sites:

1) Cholinergics and anticholineesterases; 2) Adrenergic drugs; 3) Antispasmodic and antiulcer drugs; 4) Neuromuscular blocking agents; 5) Eicosanoids; 6) Analgesic, Antipyretics, Antiinflammatory (Non steroidal) agents.; 7) DIURETICS, ANTICOAGULANT AND ANTIPLATELET DRUGS AND CARDIOVASCULAR DRUGS Oxytocics (including Oxytocin, ergot alkaloids and prostaglandins), Biochemical approaches in drug

designing wherever applicable should be discussed.

Elective 2

Spectroscopy and Computation Applications in Modern Chemistry (Same as PhD course work CY31101)

Module 1:

Details of UV-vis and IR spectroscopy. Principle and application in interpretation of organic functional groups, Woodward-Hoffman rule. ^{1}H NMR Spectroscopy: Basic theory – phenomenon of energy absorptions (resonance) and relaxation, chemical shift, shielding and de-shielding mechanisms, equivalence and nonequivalence of protons, spin-spin coupling – notation for spin systems, coupling constant and its variation with stereochemistry - Karplus equation. 13C NMR Spectroscopy: Principles; broadband decoupling, DEPT.

Module 2:

Mass Spectrometry: Types of ionization techniques, basic principles of EI. Fragmentation processes and structural analysis; ESI, GC/MS, LC/MS and MS/MS techniques, fragmentation pattern of small molecules and interpretation of spectroscopic (NMR, IR and mass) data, as applied to organic, inorganic and biological systems

Module 3:

Introduction to 2D NMR: NOESY, COSY, HETCOR, HOMCOR, INADEQUATE, INDOR, INEPT for simple compounds and problems. Applications of multinuclear NMR in inorganic compounds – Examples from 1H, 11B, 13C, 19F, 15P NMR of paramagnetic molecules – Lanthanide shift.

Module 4:

Concept of vector space, matrix representation of operators, Hermitian operators and matrices, solutions of eigenvalue equation. Comparison between Schrodinger and Heisenberg pictures. Born-Oppenheimer approximation, theories of valence, the MO and VB methods for H2 molecule – their relative merits, dissociation curve, excited state, configuration interaction. Many electron systems – its characteristics, independent particle model (IPM), Hartree and Hartree- Fock methods for closed shell (elementary ideas).

Elective 3

Synthetic Methodologies & Applications in Chemistry (Same as PhD coursework CY31102)

Module I: Development of methodology

Advance reagents used as catalyst, oxidizing agent, reducing agent, Application to chemical transformation.

Module II: Supra molecular chemistry

Host guest chemistry, Design and synthesis of supramolecular architecture, Practical application of supra molecular chemistry.

Module III: Asymmetric synthesis

Introduction of chirality, Stereo selective & Stereospecific Synthesis, carbohydrate chemistry and functional group transformation.

Module IV: Organocatalyst in organic synthesis

Design of organocatalyst and application to develop new asymmetric transformations.

Elective 4

MOLECULAR CATALYSTS FOR WATER OXIDATION

Module 1

Role of water oxidation in Energy Storage; Natural Photosynthetic Water Oxidation; Water Electrolysis.

Module 2

Heterogeneous oxide-based catalysts. Molecular Catalysts for Water Oxidation;

Module 3

Mechanistic investigation regarding O-O bond formation pathways (Water Nucleophilic Attack, WNA mechanism; Interaction of two M-O units, 12M etc). Deactivation pathways.

Module 4

Selected examples of Manganese based catalysts; Ruthenium based catalysts; Iridium based catalysts; Iron based catalysts; Cobalt based catalysts; other catalysts; Challenges and future direction.

Elective 5

Inorganic Photochemistry

Module 1

Introduction to inorganic photochemistry. Photochemical laws and photochemical kinetics. Photophysical processes.

Module 2

The electronic absorption spectra of inorganic compounds. Characteristics of the electronically excited states of inorganic compounds. Photoelectochemistry of excicted state redox reactions.

Module 3

Photosensitization. Photochemical reactions; substitution, decomposition and fragmentation, rearrangement, and redox reactions.

Module 4

Selective inorganic photochemistry using laser beams. Inorganic photochemistry in biological processes and their model studies.

Text/References

G. L.Geoffrey and M. S. Wrighton, Organometallic Photochemistry, Academic Press, 1979.
K. K. Rohatagi-Mukherjee, Fundamentals of Photochemistry, Wiley Eastern, 1978.
M. S. Wrighton, Inorganic and Organometallic Photochemistry, ACS Pub.,1978.
V. Balzani and V. Carasiti, Photochemistry of Co-ordination compounds, Academic Press, 1970.

Elective 6

Determination of Molecular Structure by X-ray Diffraction

Module 1

Generation of X-rays, monochromators, safety; Concept of direct and reciprocal lattices, Bragg's law of X-ray diffraction in direct and reciprocal lattice, crystal systems, point groups

Module 2

Bravais lattices; Rotational axes of symmetry, screw axes, glide planes, equivalent points, systematic absences, space groups

Module 3

Argand diagram, intensity data collection and quantitative aspects of X-ray diffraction, temperature factor and scaling of data.

Module 4

The phase problem, direct method of solving structures; Patterson method, isomorphous replacement method; Structure refinement and their critical evaluation.

Elective 7

Frontiers in Bioinorganic Chemistry

Module 1

Developing facets of Inorganic Chemistry; Oxidative generation of molecular oxygen from water during photosynthesis; Its importance from the standpoint of non-conventional energy research;

Module 2

Reductive cleavage of the dioxygen bond; Reductive cleavage of dioxygen bond and novel organic transformations including methane to methanol performed by a large number of Fe containing metalloenzymes;

Module 3

Reductive cleavage of dioxygen bond and novel organic transformations performed by a large number of Cu containing metalloenzymes and synthetic catalysts.

Elective 8

The Chemistry of Metal-Carbon Bond: Structure Reactivity & Applications

Module 1

Introduction to Organometallics: Bonding, Types of Ligands, and some basics concepts like isoelectronic and isolobal analogy; Characterization techniques of Organometallic compounds (NMR and IR spectroscopy and Mass spectrometry);

Module 2

Representative chemistry of main group Organometallics; Organometallic chemistry of lithium and magnesium: synthesis, structures, fluxionality and reactivity; Chemistry of Aluminum: Aluminum alkyls. Use of aluminum alkyls in polymerization of olefins;

Module 3

Organometallic chemistry of transition metals σ – bondedligands: Metal alkyls, aryls and hydrides. Stability, preparation and reactivity; Metal- carbonyls / Metal- phosphines / metal- nitrosyls / metal isocyanide: structures, reactivity and bonding; Metal- carbenes, metal-carbynes, Fischer carbenes, Schrock, carbenes, complexes with N-heterocyclic carbenes (NHCs), π - bonded ligand:

Module 4

Metal-olefins, alkyls metal alkynes, dienes, Cp and Cp*, structure, bonding and reactivity. Reactions in Organometallic Chemistry: Oxidative addition, reductive elimination, insertion, elimination, and migration; Applications of organometallics in organic synthesis; C-C bond coupling reactions (Heck, sangoshira, Suzuki); Reduction using transition metal hydrides, asymmetric hydrogenation. Olefin metathesis

Elective 9

Solid-State Chemistry

Basic Principles and applications Solid State Reactions: General Principles, Experimental procedure, Kinetics of solid-state reactions, Synthesis of Single Crystals, Phase transitions, electronic and magnetic properties Factors that influence kinetics of phase transition. Electronic Properties and Band Theory: Electronic structure of solids-band theory. Magnetic Properties: Classification of materials. Magnetism: Types, determination of magnetic susceptibility. Quantum theory of paramagnetism. Cooperative phenomena. Magnetic domains. Hysteresis.

Diffractions Techniques X-ray Diffraction: Diffraction of X-rays by crystals: The Laue equations and Bragg's law. X-ray diffraction experiments: The powder method and the single crystal method. Electron diffraction: Scattering intensity versus scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Neutron diffraction: Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cells.

High-Tc Oxide Superconductors Structural features of cuprate superconductors. 1-2-3 and 2-1-4 cuprates; structure. Non-linear materials: Second and third order non-linear effects; molecular rectifiers. Photochromic materials; optical data storage, memory and switches.

Elective 10

Advanced Physical Chemistry

Tunnelling Phenomena: Principles and selected problems. Ab initio and Semi-empirical Methods for Closed Shell Systems: The Hartree-Fock Self-Consistent Field Method: The generation of Optimized orbitals, Koopman's Theorem. Density matrix analysis of the Hartree-Fock Approximation, Natural orbitals, The matrix solution of the Hartree- Fock Equations (Roothaan's equations). Density functional theory. Semiempirical Molecular Orbital Methods I - PI Electron Systems: The Hückel Approximation for Conjugated Hydrocarbons, The Pariser-Parr-Pople Method. Semiempirical Molecular Orbital Methods II - All valence - Electron systems: The Extended Hückel Method, The CNDO Method.

Electronic Structure of Linear and non linear Molecule The MO - LCAO Approximation, The Hydrogen Molecule Ion, H_2^+ , The Hydrogen molecule, Molecular Configuration - Interactions, The Valence Bond Method, Molecular Perturbation Calculations. Electronic Structure of AH_n molecule: Methane, Ammonia and Water, Hybrid Orbitals: The Ethylene and Benzene Molecules.

Elective 11

Nanoscience

Introduction Surface to volume ratio, crystal structures, basic properties. Length scale: de Broglie wavelength, Bohr radius, excitons, confinement regimes, The Fermi Energy, Kubo Gap, the mean free path in metals, charging energy. Size and shape-dependent electrical, magnetic and optical properties of metal, metal oxide and semiconductor nanoparticles. Quantum size effect, Superparamagnetism, Surface Plasmon resonance.

Synthetic approaches Top down and bottom up. Colloidal growth. Chemical synthesis, functionalisation and basic characterisation of metal, metal oxide and semiconductor nanoparticles. Core-shell / multishell nanoparticles. Properties and synthesis of Carbon nanotubes, grapheme, fullerene. Recent advances in synthesis of new materials and their synthetic strategies. Characterization of nanomaterials.

Polymer-nanoparticle composite. Band gap engineering in semiconductor nanocrystals, Carbon based nanoparticles, self assembled nanostructures. Atom and molecule manipulation. Application of nanoparticles in drug delivery, biological imaging of cellular and subcellular structures, catalysis, sensor, tracer, cancer treatment, photovoltaics, single molecule detection and LED. Introduction to nanotoxicology. Model problems for quantum wells, wires and dots Density of states.

Elective 12

Advanced Materials

Glasses, ceramics, composites and Nano materials. Glasy state, glass formers and modifiers, applications, ceramic structures, mechanical properties, clay products, refractories, characterization, property and application. Preparation, characterization, properties, applications of nanomaterials.

Thin Films and Langmuir – Blagett films: Preparator techniques, chemical, MOCVD, sol-gel etc. CB films, growth technique, Properties and applications. Liquid Crystals: Mesomorphic behavior, different phases in liquid crystals order parameters, textures, twisted and chiral nematics, chiral nematics, application of liquid crystals.

Fullerenes, Graphene, Carbon Nanotubes, Metal Organic Frameworks.

Elective 13

Computational Chemistry

Monte Carlo, Molecular Dynamics simulations and its applications to understanding of physical and chemical transformations Methods based on Hartree-Fock, Configuration Interaction, Deriving one and two electron properties, Semi-empirical methods, Coupled Cluster theory, Density functional theory, TDDFT. QM/MM methods. Basic molecular biology Basic principles of biochemistry, energy conversion, enzymatic catalysis, and active transport, enzyme models, drug design, computational modeling. Introduction to Classical Monte Carlo Molecular Dynamics Simulation and Softwares - DLPOLY, GROMACS, TOWHEE, NAMD. Introduction to Quantum chemistry softwares – NwChem, Gaussian.Visualization softwares – VMD, Povray. Computer programming languages C++, FORTRAN. Python, Shell scripting. Writing Monte Carlo, Molecular Dynamics codes for chemistry problems. Parallel programming techniques like Open MP, MPI