# BSc Honors in Chemistry Degree Program

## Faculty of Science University of Kelaniya BSc Honors in Chemistry Degree

Level	<b>Course Code</b>	Course Title	Status
	CHEM 44704	Advanced Analytical Chemistry	С
	CHEM 44714	Advanced Biochemistry I	C
	CHEM 44723	Advanced Inorganic Chemistry I	С
	CHEM 44733	Advanced Organic Chemistry I	С
	CHEM 44743	Advanced Physical Chemistry I	С
Linivansity	CHEM 44753	Analytical and Environmental Chemistry Laboratory	С
University Level 3	CHEM 44762	Biochemistry Laboratory	С
Level 3	CHEM 44772	Inorganic Chemistry Laboratory	С
	CHEM 44782	Organic Chemistry Laboratory	C
	CHEM 44792	Physical Chemistry Laboratory	C
	CHEM 44802	Applications in Computational Chemistry	C
	CHEM 44811	Industrial/ Professional Placement <sup>1</sup>	C
	CHEM 44821	Seminar	C
	CHEM 44832	Earth Resources and Smart Materials	C
	CHEM 44843	Advanced Biochemistry II	C
	CHEM 44854	Advanced Environmental Chemistry	C
T.T. ::4	CHEM 44863	Advanced Inorganic Chemistry II	C
University Level 4	CHEM 44874	Advanced Organic Chemistry II	C
Level 4	CHEM 44884	Advanced Physical Chemistry II	C
	CHEM 44893	Chemical Engineering and Management Concepts in	C
		Industrial Chemistry	
	CHEM 44902	Food Chemistry	С
	CHEM 44912	Polymer Chemistry	С
	CHEM 43928	Research Project/ Dissertation	С

<sup>&</sup>lt;sup>1</sup>Credit not counted for the GPA Calculation

## **University Level 3**

Semester	1 or 2				
Course Code	CHEM 44704				
Course Name	Advanced Analytical Cl	nemistry			
Credit Value	4				
Compulsory/ Optional	Compulsory				
Pre- requisites		-			
Co- requisites		-			
Hourly Breakdown	Theory Practical Independent Learning				
	60	-	140		

## Course Aim/ Intended Learning Outcomes:

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

- explain the function of the components of instruments and capabilities and limitations in their analytical applications
- explain the importance of the effects of the experimental conditions in analysis and modify the method used or correct the data accumulated using their knowledge of conditional parameters
- use the knowledge in fundamentals to design analytical methodologies for analyzing of samples with complex matrices
- apply advanced analytical techniques based on electrochemistry, spectroscopy and separation & thermal methods in analyzing complex samples

#### **Course Content:**

## Principles of Instrumentation (10 h)

Instrument performance characteristics; UV-visible spectrometers, atomic spectrometers, Fourier transformed infrared spectrometers, gas chromatographs and high performance liquid chromatographs, mass spectrometers. Analytical measurements; quality assurance and quality control in measurements. Signals, noise and signal to noise ratio. Basic operational amplifier circuits and their applications. Data quality and reporting.

#### Analytical Electrochemistry (10 h)

Controlled potential microelectrode techniques; potential step methods and potential sweep methods. Controlled current microelectrode techniques. Methods involving forced convection. Hydrodynamic methods. Techniques based on concept of impedance. Electrochemical quartz crystal micro and nano balance techniques.

#### Analytical Spectroscopy and Radiochemical Methods of Analysis (10 h)

Inductively coupled plasma mass spectrometry, laser ablation in atomic spectrometry. Microwave induced plasma systems for atomic spectrometry. X-ray fluorescence spectrometry, γ-spectrometry and neutron activation analysis.

## Complex Chemical Equilibria (10 h)

Importance of conditional equilibrium constants and non-ideal systems, activity and activity coefficients, conditional solubility product and its application in non-ideal systems, acid-base equilibria in polyprotic systems, conditional constants in complexometry, redox and precipitation titrations. Non aqueous solvents and their applications in chemical analysis, speciation, importance and difficulties in analysis.

## Analytical Separations (14 h)

Solvent extraction, distribution constant and distribution ratio, conditional effects on the efficiency of analytical separations, chromatography; concepts, terms, definitions and tools used, gas chromatography (GC), high performance liquid chromatography (HPLC), capillary electrophoresis (CE), ion exchange chromatography (IEC), method development in separation analysis.

## Thermal Methods in Chemical Analysis (6 h)

Definitions & tools used in thermal analysis, thermo-gravimetric analysis (TGA), differential thermal analysis (DTA), differential scanning calorimetry (DSC), temperature programmed reduction (TPR) & temperature programmed oxidation (TPO), combustion analysis, thermo mechanical analysis (TMA), thermometric titrations.

**Teaching/ Learning Methods:** A combination of lectures and tutorial discussions (supporting materials will be provided via Computer Assisted Learning (CAL))

## **Assessment Strategy:**

Continuous assessment and end of semester examination.

	Continuous Assessment	Final Assessment		
Details	20%		80%	
2 Cums	Quizzes/ Assignments	Theory	Practical	Other
	20	80	-	-

- 1. Harris, D.C., Lucy, C.A., (2020) Quantitative Chemical Analysis, Macmillan.
- 2. Skoog, D.A., James F.H., Nieman. T. A., (2018) *Principles of Instrumental Analysis*, Harcourt Brace College Publishers.
- 3. Skoog, D.A., Donald M. W., James, F.H., (2014) *Fundamentals of Analytical Chemistry*, Saunders College Publishing.
- 4. Paul, M.S. Monk., (2001) Fundamentals of Electroanalytical Chemistry, Wiley.
- 5. Willard, H.H., Merritt, L., Dean, J., Settle, F., (2004) *Instrumental Methods of Analysis*, Wadsworth.
- 6. Flaschka, H.A., Barnard, A.J., Sturrock, P.E., (1969) *Quantitative Analytical Chemistry*, Vol 1, Barnes & Noble.
- 7. Mendham, J., Denney, R.C., Barnes, J.D., (2002) *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson.
- 8. Currel, G., (2010) *Analytical Instrumentation: Performance Characteristics and Quality*, John Wiley & Sons, Ltd.

Semester	1 or 2				
Course Code	CHEM 44714				
Course Name	Advanced Biochemistry	· I			
Credit Value	4				
Compulsory/ Optional	Compulsory	Compulsory			
Pre- requisites		-			
Co- requisites		-			
Hourly Breakdown	Theory Practical Independent Learning				
	60	-	140		

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

- describe theoretical and practical aspects of advanced enzyme kinetics
- describe the structure, dynamics, interactions, and functions of biological systems at molecular level
- appraise biophysical methods in modern biomolecular research and technology
- demonstrate the knowledge of the importance of biomolecular modeling in designing novel drugs in pharmaceutical research
- perform computer simulations to manipulate, and optimize 3D models of biomolecules using various software in a laboratory environment

#### **Course Content:**

#### Advanced Enzyme Kinetics (20 h)

The steady state of an enzyme-catalyzed reaction. The Briggs-Haldane treatment. The reversible Michaelis - Menten mechanism. Practical aspects of kinetic studies. Inhibition and activation of enzymes; catalytic poisons, types of reversible inhibition, linear inhibition, specific inhibition, mixed inhibition, competitive inhibition, hyperbolic activation and inhibition. Multi substrate system. Fast reaction; Burst kinetics. Active site titration analysis of enzyme kinetic data. Use of isotopes for studying enzyme mechanism.

### Biophysics (20 h)

Three-dimensional structure of proteins; amino acids, peptides, protein structure, protein folding, protein denaturation. Protein function; reversible ligand binding to proteins (oxygen binding proteins). Conformations of macromolecules; Molecular associations, co- operativity, allosteric interactions. Protein sequences and evolution. Biomechanics; conversion of chemical energy to mechanical force (actin, myosin and molecular motors). Biological membranes and transport; membrane composition and architecture, membrane dynamics, solute transport across membranes (diffusion and Brownian motion, ion permeation and membrane potential). Cellular homeostasis.

Physical methods for determination of macromolecular structures; CD, NMR spectroscopy (COSY, TOCSY and NOESY NMR techniques), X-ray crystallography.

## Molecular Modeling (20 h)

Concept of molecular modeling; force field models, energy landscapes and minimization methods, computer simulation methods, molecular dynamics simulation methods, Monte Carlo simulation. Protein structure prediction; sequence analysis and protein folding, protein secondary structure prediction and 3D structure modeling, protein 3D structure visualization, conformational analysis. 3D structure alignment, protein-protein and protein-ligand docking free energy calculations through simulations. Pharmacoinformatics to discover and design new drugs.

**Teaching/ Learning Methods:** A combination of lectures, take-home assignments, in-class assignments and group discussions, tutorial discussions and problem-based learning (in-class computer laboratory sessions, supporting materials will be provided via CAL).

## Assessment Strategy:

Continuous assessment and end of semester examination.

	Continuous Assessment		Final Assessment	
Details	20%		80%	
Betans	Quizzes/ Assignments	Theory	Practical	Other
	20	80	-	-

- 1. Nelson, D. L and Cox, M.M., (2017), Lehninger *Principles of Biochemistry*, W.H. Freeman.
- 2. Freshet A., (1993), Enzyme Structure and Mechanism, Freeman.
- 3. Arrondo J.L.R., Alonso A, (2006), *Advanced Techniques in Biophysics*, Springer-Verlag, Heidelberg.
- 4. Holtje et al., (2008), *Molecular Modeling, Basic Principles and Applications*, Wiley-VCH Verlag GmbH & Co.

Semester	1 or 2				
Course Code	CHEM 44723				
Course Name	Advanced Inorganic Ch	emistry I			
Credit Value	3				
Compulsory/ Optional	Compulsory	Compulsory			
Pre- requisites		-			
Co- requisites	-				
Hourly Breakdown	Theory Practical Independent Learning				
	45	-	105		

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

- describe and explain electronic spectra, highlighting the atomic/ molecular level structural and environmental features
- explain and postulate reaction mechanisms for inorganic reactions using experimental data and structural features of compounds involved
- explain and postulate reaction mechanisms for organometallic reactions using the knowledge of transition metal based organic compounds
- describe structural information based on X-ray crystallographic data

## Course Content:

#### Spectral and Magnetic Properties of Inorganic Compounds (11 h)

Spectral properties of coordination compounds; electronic spectra, types of transitions, term symbols, micro energy states and ground state determination, Russell-Saunders coupling, Orgel energy diagrams of transition metal complexes, Racah parameters, non-crossing rule, Tanabe-Sugano energy diagrams. Charge transfer transitions in metal complexes. Magnetic properties of transition metal compounds.

#### Inorganic Reaction Mechanisms (11 h)

Reaction kinetics and mechanism; stoichiometric and intimate mechanisms, ligand substitution reactions of inorganic complexes, associative and dissociative pathways, ligand exchange reactions of square planner complexes; rate law mechanisms, factors controlling the rate of square planner substitutions, trans effect theories, trans influence, cis-effect. Substitution reactions of octahedral complexes; rate law mechanisms, rates of water exchange, study of acid hydrolysis, base hydrolysis and anation reactions, stereochemical changes in substitution reactions. Electron transfer processes; outer-sphere and innersphere mechanisms; Frank-Condon factors, factors affecting inner-sphere reactions.

#### Crystallography (11 h)

Space groups, X-ray diffraction, single crystal method and powder diffraction method, application of x-ray crystallography, x-ray diffraction patterns in one, two and three dimensions, the structure and the atomic structure factor, the phase problems, direct methods for solving phase problem, the Patterson maps, isomorphous replacement, model building, refinement and evaluation of models.

#### Chemistry of Organotransition Metal Compounds: Bonding to Catalysis (12 h)

Molecular orbital theory of metal- ligand bonding, bonding properties of ligands like allyl, arenes, cyclopentadinenes, carbenes, phosphines, etc. Ligand effects on transition metal complexes, Reactivity of organometallic compounds; nucleophilic and electrophilic attack on coordination ligands, σ-bond

metathesis, migratory insertion, transmetallation etc., homogeneous catalysis and catalytic cycles; Alkene metathesis, Hydrogenation of alkenes, C-C coupling reactions etc.

**Teaching/ Learning Methods:** A combination of lectures and tutorials (supporting materials will be provided via CAL)

#### **Assessment Strategy:**

Continuous assessment and end of semester examination.

	Continuous Assessment		Final Assessment	
Details	20%		80%	
Betains	Quizzes/ Assignments	Theory	Practical	Other
	20	80	-	-

- 1. Miessler, G. L., Fischer, P. J., Tarr, D.A. (2014), *Inorganic Chemistry*, Pearson.
- 2. Crabtree, R. H. (2019), The Organometallic Chemistry of the Transition Metals, Wiley.
- 3. Hartwig, J. F. (2010), Organotransition Metal Chemistry: From Bonding to Catalysis, University Science Books.
- 4. Sharpe, A.G., (2002) Inorganic Chemistry, Pearson
- 5. Cotton, F.A., Wilkinson, G., Murillo, C. A, Bochmann, M; (2007), *Advanced Inorganic Chemistry*, New York, John Wiley.
- 6. Lee, J.D., (2008) Concise Inorganic Chemistry, Blackwell
- 7. Prakash, S., Basu. S.K., Tuli. G.D. and Madan.R. D., (2013) *Advanced Inorganic Chemistry*. Vol (II) Chand.
- 8. Atkins, P. W., De Paula, J., Keeler, J., (2017) *Physical Chemistry*, Oxford.
- 9. Ladd, M. F. C. and Palmer, R. A., (2013) *Structure Determination by X-ray Crystallography*, Springer.

Semester	1 or 2			
Course Code	CHEM 44733			
Course Name	Advanced Organic Che	mistry I		
Credit Value	3			
Compulsory/ Optional	Compulsory			
Pre- requisites		-		
Co- requisites	-			
Hourly Breakdown	Theory Practical Independent Learning			
	45	-	105	

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

- apply thermodynamic and kinetic concepts to interpret organic reactions
- apply advanced spectroscopic techniques for structure elucidation of organic compounds
- explain theoretical basis of advanced techniques in Nuclear Magnetic Spectroscopy and Mass Spectrometry
- design suitable retrosynthetic pathways for target molecules
- select the most appropriate reaction conditions and reagents for a particular synthetic process.

#### **Course Content:**

#### Physical Organic Chemistry (15 h)

Stereochemical principles; stereospecific and stereoselective reactions, dynamic stereochemistry, prochiral relationships, homotopic and heterotopic nuclei, enantiotopic, diastereotopic relationships. Reaction mechanisms; thermodynamic and kinetic data, substituent effects and linear free energy relationships, Hammett equation, reaction constants and substituent constants, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, isotope effects, nucleophilic substitution, quantitative measurements of the stabilities of cations, heat of ionization measurements, nucleophilicity and solvent effects, leaving groups, steric effects, substituent effects, neighboring group participation, norbornyl and other non-classical carbocations. Detailed mechanistic aspects of S<sub>N</sub>2, S<sub>N</sub>1, E1, E2, E1cb reactions. Chemistry of carbanions: acidity of hydrocarbons, kinetic and thermodynamic acidity, Free radicals; stable free radicals, persistent free radicals etc., free radical reaction mechanisms.

#### Advanced Organic Spectroscopy (15 h)

Principles of pulsed Fourier transform spectrometry, instrumentation, non-first order spectra, effect of magnetic field on resolution of NMR spectra, simplification of complex spectra (shift reagents), nuclear overhauser effect (NOE), DEPT, <sup>1</sup>H-<sup>1</sup>H COSY, HMQC, HMBC and HMBC, mass spectrometry; components in modern mass spectrometers, ionization methods (EI, CI, FAD, ESI, MALDI etc), mass analyzers (magnetic sector, quadrupole analyzer, FTICR, TOF etc.), detection of molecular formula using high resolution molecular ion, interfacing of MS with GC (GCMS) and LC (LCMS), fragmentation patterns of some chemical classes of organic compounds. Other methods; use of FTIR, CD and ORD in structure elucidation of organic compounds.

## Advanced Organic Synthesis (15 h)

Strategies and tactics in organic syntheses; retrosynthesis, transformations, disconnections and

synthons. Strategies in ring syntheses (5 and 6 membered compounds), use of non-nucleophilic bases, strategies in controlled alkylations, reactions of  $\alpha$ -thiocarbanions. Applications and methods of reversal of the polarity. Applications of Wittig reaction, Diels-Alder reaction, Mannich reaction, Baeyer-Villiger oxidation, oxidation of tertiary allylic alcohols, use of alpha methoxyvinyl lithium and organocopper reagents in retro-syntheses. Application of protecting groups (for alcohols, carbonyl compounds, carboxylic acids and amines) in linear and convergent syntheses.

**Teaching/ Learning Methods:** A combination of lectures and tutorials (supporting materials will be provided via CAL)

#### **Assessment Strategy:**

Continuous assessment and end of semester examination.

	Continuous Assessment		Final Assessment	
Details	20%		80%	
Betans	Quizzes/ Assignments	Theory	Practical	Other
	20	80	-	-

- 1. Firebolin, H., (2004) Basic One and Two Dimensional NMR Spectroscopy, VCH.
- 2. Silverstein, R.M., Webster, F. X., (1997) *Spectrometric Identification of Organic Compounds*, John Willey.
- 3. Sanders, J. K. M. and Hunter, B. K., (1993) *Modern NMR Spectroscopy*, Oxford University Press.
- 4. Williams, D. and Fleming I., (1989) *Spectroscopic Methods in Organic Chemistry*, McGraw-Hill International (UK) limited.
- 5. Thomas, S.E., (1991) *Organic Synthesis: The Role of Boron and Silicon*, Oxford Chemistry Primers.
- 6. Jenkins, P.R., (1992) Organometallics Reagents in Synthesis, Oxford Chemistry Primers.
- 7. Carruthers, W., (1996) *Modern Aspects of Organic Synthesis*, Cambridge press.
- 8. Carey, F. A., Sundberg, R. J., (2007) *Advanced Organic Chemistry Part A: Structure and Mechanisms*, Springer.

Semester	1 or 2				
Course Code	CHEM 44743				
Course Name	Advanced Physical Che	emistry I			
Credit Value	3	3			
Compulsory/ Optional	Compulsory				
Pre- requisites		-			
Co- requisites	-				
Hourly Breakdown	Theory Practical Independent Learning				
	45	-	105		

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

- summarize the principles and concepts used to analyze thermodynamic systems and processes
- determine the wave functions, energy eigenvalues and other observables for simple quantum mechanical systems using models to represent translation, rotation and vibration of atoms
- explain the use of approximation methods to solve complex quantum mechanical systems
- use theories to identify, formulate, and solve problems related to chemical kinetics
- use basic aspects of group theory to describe molecular orbitals of small molecules and coordination complexes
- use group theory to generate and factor reducible representations for molecular vibrations, rotations, translations

## **Course Content:**

## Advanced Thermodynamics (10 h)

Material equilibrium, chemical potential, partial molar quantities, mixing quantities, thermodynamic properties of ideal solutions, standard thermodynamic functions of reaction, multiphase closed systems, phase equilibrium and reaction equilibrium in ideal gas mixtures, conventional entropies and the third law of thermodynamics.

### Advanced Quantum Mechanics (12 h)

Schrodinger equation and its applications, solutions for particle in a box model, rigid rotor model and simple harmonic oscillator model, Pauli exclusion principle, spatial and spin parts of wave function, Schrodinger equation for molecules, tunneling, many electron atoms, approximation methods: Born-Oppenheimer approximation, variational method, perturbation theory

#### Advanced Reaction Kinetics (12 h)

Review of fundamental laws of kinetics. Theories of reaction rates; collision theory and activated complex theory, Eyring equation, thermodynamic parameters, potential energy surfaces. Theories of unimolecular reactions; Lindemann theory, Hinshelwood theory and Kassel's modifications of Lindemann theory, liquid phase reactions, diffusion controlled and activation-controlled reactions and determination of reaction rates.

## Symmetry and Group Theory (11 h)

Determination of point groups, set up a matrix to perform a given transformation, reducible and irreducible representations, character tables, application of group theory in chemical bonding and molecular spectroscopy.

**Teaching/Learning Methods:** A combination of lectures and tutorials (supporting materials will be provided via CAL)

#### **Assessment Strategy:**

Continuous assessment and end of semester examination.

	Continuous Assessment		Final Assessment	
Details	20%		80%	
2 Cums	Quizzes/ Assignments	Theory	Practical	Other
	20	80	-	-

- 1. Levine, I. N., (2011) Physical Chemistry, McGraw-Hill.
- 2. Atkins, P. W., (2018) Physical Chemistry, Oxford.
- 3. McQuarrie, D. A. (1997), *Physical Chemistry: A Molecular Approach*, University Science Books.
- 4. Price, G., (1998) Thermodynamics of Chemical Processes, Oxford.
- 5. Atkins, P. W., Friedman, R. S, (2010) Molecular Quantum Mechanics, Oxford University Press.
- 6. Levine, I. N., (2013) Quantum Chemistry, Prentice-Hall, Inc.
- 7. Laidler. K. J., (2003) Chemical Kinetics, Pearson.
- 8. Pilling. M. J., Seakins. P. W., (1996) Reaction Kinetics, Oxford.
- 9. Cox. B. G., (1994) Modern Liquid Phase Kinetics, Oxford.
- 10. Brouard. M., (1998) Reaction Dynamics, Oxford.
- 11. Sharp A. G., Housecroft C., (2018), Inorganic Chemistry, Pearson.

Semester	1 or 2				
Course Code	CHEM 44753	CHEM 44753			
Course Name	Analytical and Environ	mental Chemistry Labor	ratory		
Credit Value	3	3			
Compulsory/ Optional	Compulsory	Compulsory			
Pre- requisites		-			
Co- requisites		-			
Hourly Breakdown	Theory	Theory Practical Independent Learning			
	-	98	52		

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

- operate common analytical instruments properly and optimize experimental conditions to achieve high sensitivity, selectivity, accuracy and reproducibility in chemical analysis
- apply analytical techniques to measure analytes in non-ideal conditions and hence will be able to analyze natural and industrial samples
- apply the knowledge in chemical principles and skills acquired in laboratory techniques to investigate chemical processes occurring in the environment and monitor pollutants in the environment

#### **Course Content:**

Calibration of glassware, direct measuring instruments and analytical instruments. Use of spectrometers; UV-visible, atomic emission and atomic absorption spectrophotometers. Electro-analytical instruments (voltammeters, ion selective electrodes) and chromatographic equipment (gas chromatograph and liquid chromatograph) for analysis of natural samples. Material analysis (Thermal and XRD.). Use of basic software packages for data processing and reporting of analytical results. Conditional effects on titrimetry and gravimetry, non-aqueous titrations.

Techniques of environmental sample collection, sample preparation and sample storage. Study of inorganic and organic chemical properties of natural and wastewaters. Study of processes of generation, propagation and transformation of environmental pollutants in the geosphere and biosphere. Introduction to speciation in environmental analysis; relationship with toxicity testing. (includes background on speciation of Hg, Pb, Cd, As, Sn) Investigations on pollution mitigation methods. Case study on applied green chemistry.

**Teaching/ Learning Methods:** Two 7- hour laboratory classes per week for 7 Weeks, pre lab quizzes and assignments (supporting materials will be provided via CAL).

#### **Assessment Strategy:**

Continuous assessment and end of semester examination.

	Continuous Asses	ssment	F	Final Assessm	ent
Details	30%		70%		
	Quizzes/ Assignments	Lab Reports	Theory	Practical	Other
	20	10	-	70	-

- 1. Reading materials (Journal articles related to experiments) will be provided during the laboratory classes.
- 2. Skoog, D.A., James F.H., Nieman. T. A., (2018) *Principles of Instrumental Analysis*, Harcourt Brace College Publishers.
- 3. Willard, H.H., Merritt, L., Dean, J., Settle, F., (2004) *Instrumental Methods of Analysis*. Wadsworth.
- 4. Harris, D.C., Lucy, C.A., (2020) Quantitative Chemical Analysis, Macmillan.
- 5. Mendham, J., Denney, R.C., Barnes, J.D., (2002) *Vogel's Textbook of Quantitative Chemical analysis*. Pearson.
- 6. Keith, L. H., (1991) Environmental sampling and Analysis. A Practical Guide, Lewis.
- 7. Azara, J. et.al. (1997) ASTM Standards on Environmental Sampling.
- 8. Radojevic, M., Bashkin, V. N., (1999) Practical Environmental Analysis, RSC.
- 9. Boehnke, D. N., Delumyea, R. D., (2000) *Laboratory Experiments in Environmental Chemistry*, Prentice Hall.
- 10. Maria, C., Saba, C., (2002) Environmental Sampling and Analysis for Metals, Lewis Publishers.
- 11. Eugene, R.W., (2000) Applications of Environmental Chemistry. A practical Guide for Environmental Professionals, CRC.

Semester	1 or 2			
Course Code	CHEM 44762			
Course Name	Biochemistry Laborator	ry		
Credit Value	2			
Compulsory/ Optional	Compulsory			
Pre- requisites		-		
Co- requisites	-			
Hourly Breakdown	Theory	Practical	Independent Learning	
	-	70	30	

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

- apply laboratory skills to isolate and manipulate native proteins from biological sources
- use bioanalytical techniques to detect, quantify and check purity of proteins
- develop methods to evaluate biological activity of enzymes and proteins
- design experiments and estimate kinetic parameters of enzymes

#### Course Content:

Protein/ enzyme extraction and purification, salting-out, protein dialysis, ion exchange chromatography, size exclusion chromatography, and affinity chromatography. SDS-PAGE. Enzyme kinetics;  $K_m$ ,  $V_{max}$ , specific activity, and enzyme inhibitors. Immuno- precipitation reactions and immunoassays.

**Teaching/ Learning Methods:** Two 7- hour laboratory classes per week for 5 Weeks, pre lab quizzes and assignments (supporting materials will be provided via CAL).

## **Assessment Strategy:**

Continuous assessment and end of semester examination.

	Continuous Assess	sment		Final Assessmen	nt
Details	30%		70%		
Details	Quizzes/ Assignments	Lab Reports	Theory	Practical	Other
	20	10	-	70	-

- 1. Reading materials (Journal articles related to experiments) will be provided during the laboratory classes.
- 2. Minch, M. M. J., (1989), Experiments in Biochemistry, Prentice Hall.
- 3. Plummer, D. T., (1987), An Introduction to Practical Biochemistry, McGraw Hill.
- 4. Robyt, J.F, White B.J., (1990), Biochemical Techniques, Theory and Practices, Waveland Press.

Semester	1 or 2			
Course Code	CHEM 44772			
Course Name	Inorganic Chemistry L	aboratory		
Credit Value	2			
Compulsory/ Optional	Compulsory			
Pre- requisites		-		
Co- requisites	-			
Hourly Breakdown	Theory	Practical	Independent Learning	
	-	70	30	

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

• apply laboratory skills and techniques to synthesize and characterize inorganic compounds.

#### Course Content:

Synthesis of air stable coordination complexes, UV- visible and IR spectroscopy of coordination complexes and characterization of coordination compounds

**Teaching/ Learning Methods:** Two 7- hour laboratory classes per week for 5 Weeks, pre lab quizzes and assignments (supporting materials will be provided via CAL).

## **Assessment Strategy:**

Continuous assessment and end of semester examination.

	Continuous Assessment		Final Assessment		
Details	30%		70%		
Detains	Quizzes/ Assignments	Lab Reports	Theory	Practical	Other
	20	10	-	70	-

- 1. Reading materials (Journal articles related to experiments) will be provided during the laboratory classes.
- 2. Mendham, J., Denney, R.C., Barnes, J.D., Thomas, M, Sivasankar B., (2009) *Vogel's Textbook of Quantitative Chemical Analysis*. Prentice Hall.
- 3. Nath, M., (2016) *Inorganic Chemistry: A Laboratory Manual*, Narosa Publishing House Pvt. Ltd.

Semester	1 or 2			
Course Code	CHEM 44782			
Course Name	Organic Chemistry Lal	ooratory		
Credit Value	2			
Compulsory/ Optional	Compulsory			
Pre- requisites		-		
Co- requisites	-			
Hourly Breakdown	Theory	Practical	Independent Learning	
	-	70	30	

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

- perform phytochemical screening for natural products
- use of modern chromatographic techniques to isolate compounds and bioassay guided fractionation
- design and perform multi-step synthesis of selected organic compounds
- use alternative methods of environmentally friendly synthesis
- elucidate structures by interpreting spectra of complex organic molecules using advanced Nuclear Magnetic Resonance spectroscopic techniques and Mass Spectrometry

#### Course Content:

Phytochemical screening of natural products; chemical tests for the detection of natural products (carbohydrates, tannins, alkaloids, glycosides, steroids, saponins, terpenes and flavonoids), semi-micro scale multi-step synthesis of organic compounds, microwave synthesis of heterocyclic organic compounds, isolation, purification, quantification and characterization of natural products using chromatographic techniques (normal and reversed phase TLC, normal and reversed phase column chromatography, gel permeation chromatography, GLC, HPLC, 1D, 2D NMR, IR, mass spectrometry etc.), bioassay guided fractionation of natural products, chemical modification and synthesis of potentially active drugs. Structure elucidation of organic compounds using NMR, IR, MS and UV.

**Teaching/ Learning Methods:** Two 7- hour laboratory classes per week for 5 Weeks, pre lab quizzes and assignments (supporting materials will be provided via CAL).

## Assessment Strategy:

Continuous assessment and end of semester examination.

	Continuous Assessment		Final Assessment		
Details	30%			70%	
	Quizzes/ Assignments	Lab Reports	Theory	Practical	Other
	20	10	-	70	-

- 1. Reading materials (Journal articles related to experiments) will be provided during the laboratory classes.
- 2. Schoffstall, A. M., Barbara, B. A., Gaddis, A., Druelinger, M.L., Schoffstall, A., Gaddis, B., Druelinger, M., (2007) *Microscale and Miniscale Organic Chemistry Laboratory Experiments*, Brooks/Cole.
- 3. Pavia, D. L., Lampman, G. L., Kriz, G.S., Engel, R. G., (2007) *Introduction to Organic Laboratory Techniques: A Microscale Approach*, Brooks/Cole.
- 4. Moting, J. R., Mofrrill, T. C., Hammond, C. N. and Neckers, D. C., (1999) *Experimental Organic Chemistry*, Freeman.
- 5. Williamson, K.L., *Macroscale and Microscale Organic Experiments*, Heath and company.
- 6. Wickramarachchi, S., (2018) Structure Elucidation of Organic Compounds Using Spectroscopy: A Workbook, Problems and Answers, College of Chemical Sciences.

Semester	1 or 2				
Course Code	CHEM 44792				
Course Name	Physical Chemistry La	boratory			
Credit Value	2	2			
Compulsory/ Optional	Compulsory				
Pre-requisites		-			
Co-requisites	-				
Hourly Breakdown	Theory	Practical	Independent Learning		
	-	70	10		

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

- reinforce concepts and exploit applications by relating the experiments to fundamental physical chemistry concepts
- explain limitations associated with data and experimental uncertainties
- develop scientific judgment and ability to innovate and think critically
- perform, analyze, and describe in writing quantitative physical measurements on chemical systems that illustrate the principles of physical chemistry

#### **Course Content:**

Advanced experiments based on thermodynamics of gases and solutions, transport properties and kinetics, thermodynamics of phase equilibrium, chemistry of surfaces, chemical equilibrium and electrochemistry.

Review the use of Excel, computer-assisted data acquisition and analysis, plotting the solutions to the 1-D and 2-D Schrödinger equation.

**Teaching/ Learning Methods:** Two 7- hour laboratory classes per week for 5 Weeks, pre lab quizzes and assignments (supporting materials will be provided via CAL).

#### Assessment Strategy:

Continuous assessment and end of semester examination.

	Continuous Assessment		Final Assessment		
Details	30%		70%		
Detains	Quizzes/ Assignments	Lab Reports	Theory	Practical	Other
	20	10	-	70	-

- 1. Reading materials (Journal articles related to experiments) will be provided during the laboratory classes.
- 2. Garland, C. W., Nibler, J. W. and Shoemaker, D. P., (2002) *Experiments in Physical Chemistry*, McGraw Hill.
- 3. Halpern, A. M., McBane. G., (2006) Experimental Physical Chemistry, Macmillan.

1 or 2			
CHEM 44802			
Applications in Compu	tational Chemistry		
2			
Compulsory			
	-		
-			
Theory Practical Independent Learning			
30	-	70	
	CHEM 44802  Applications in Compute 2  Compulsory  Theory	CHEM 44802  Applications in Computational Chemistry  2  Compulsory  -  Theory Practical	

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

- explain the knowledge of the basic concepts underlying different methods in computational chemistry
- apply the knowledge of structure calculation methods
- apply the knowledge of selecting a proper basis set for a given problem
- explain the knowledge of the concepts of force field and molecular mechanics
- explain the knowledge of the theoretical aspects of a simulation performed using Monte Carlo and Molecular dynamics
- use several modeling and visualization packages (GAUSSIAN, GROMACS, VMD)
- use online resources and databases (RCSB PDB, PubChem)

## **Course Content:**

#### Electronic Structure Calculations (10 h)

Basics of quantum mechanics (QM) and atomic structure: Hydrogen atoms, Atomic units, Approximate methods, many electron systems, Born-Oppenheimer approximation, Variation and perturbation method, Spin orbitals. Hatree-Fock calculations: Hatree products, Slater determinants, Hatree-Fock approximation, Hatree-Fock equations. Basis sets: Basis set approximation, Minimal basis sets, Scaling the orbital by splitting the minimal basis set, Extended basis sets. Electron correlation: Configuration interactions, Coupled cluster method, Density functional theory (DFT) and Semi-emperical methods:  $\pi$ -methods; Valence electron methods, Extended Hückel, Use of DFT in quantum chemistry, Kohn-Sham equations, Exchange functionals, Correlation functionals, Hybrid functionals. Solvation models: Explicit models, Implicit models, hybrid models.

Hands on experiments using GAUSSIAN software: Small molecule geometry optimization, Transition states, NMR chemical shift calculations.

#### Molecular Force Fields and Molecular Mechanics (10 h)

Molecular force fields: Force fields, Potential energy functions, Inter and intramolecular interactions, Empirical parameters. Molecular mechanics (MM): MM calculations, Energy minimization, Conformational analysis, Vibrational frequencies, Normal mode analysis. Combined QM/MM methods: Solvation and solvent effects, Protein-ligand interactions.

#### Monte Carlo and Molecular Dynamics Simulations (10 h)

Monte Carlo (MC) simulations: MC integration and Markov chains, Metropolis method, Biased MC, Concept of the ensemble. Molecular dynamics (MD) simulations: Equations of motion and force calculations, Finite difference methods, Constraint dynamics, Temperature control, Calculation of properties from MD trajectories. Liquid water: models and properties.

Hand on experiments using GROMACS software package and VMD: Biomolecule simulations, Trajectory analysis

**Teaching/ Learning Methods:** A combination of lectures and tutorials (supporting materials will be provided via CAL)

## **Assessment Strategy:**

Continuous assessment and end of semester examination.

	Continuous Assessment	Final Assessment		
Details	20%	80%		
Betans	Quizzes/ Assignments	Theory	Practical	Other
	20	80	-	-

- 1. Leach, A. R., (2001) Molecular Modeling Principles and Applications, Prentice Hall.
- 2. Cramer, C. J., (2004) Essentials of Computational Chemistry, Theories and Models, Wiley.
- 3. Allen, M. P., Tildesley, D.J., (1987) Computer Simulation of Liquids, Oxford University Press.
- 4. Atkins, P. W., and Friedman, R. S., (1997) *Molecular Quantum Mechanics*, Oxford University Press.
- 5. Frenkel, D. Smit, B., (2001) *Understanding Molecular Simulation*, Academic Press.
- 6. Lewars, E. G., (2016) Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Springer.

Semester	1 or 2				
Course Code	CHEM 44811 (Credit n	CHEM 44811 (Credit not counted for the GPA calculation)			
Course Name	Industrial/ Professional	Industrial/ Professional Placement			
Credit Value	1	1			
Compulsory/ Optional	Compulsory	Compulsory			
Pre- requisites		-			
Co- requisites		-			
Hourly Breakdown	Theory Practical Independent Learning				
	-	-	50		

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

- use laboratory skills in industrial applications
- accumulate work place skills that will help them in their future careers

#### **Course Content:**

The students will be placed in selected industries and institutions which carryout chemistry related work/research for a period of six weeks. The required resource material will be supplied by the relevant institution/ industry.

**Teaching/ Learning Methods:** Self-study, small group discussion and through feedback from appointed academic staff member.

#### **Assessment Strategy:**

Evaluation of the progress report submitted by the trainee.

Continuous Assessment	Final Assessment
100%	-

## Reading Material:

1. Research papers, review articles, textbooks related to the work carried out in the industry/ research institute..

Semester	1 or 2		
Course Code	CHEM 44821		
Course Name	Seminar		
Credit Value	1		
Compulsory/ Optional	Compulsory		
Pre- requisites		-	
Co- requisites		-	
Hourly Breakdown	Theory	Practical	Independent Learning
	-	-	50

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

 develop knowledge and presentation skills in delivering a scientific seminar on a selected topic

#### **Course Content:**

Search, select and gather information on a given topic based on a review article selected by an academic staff member. Make a suitable presentation and present to an audience of academics.

**Teaching/ Learning Methods:** Self- study, small group discussion and feedback from appointed academic staff member.

## **Assessment Strategy:**

Seminar presentation and oral examination

Continuous Assessment	Final Assessment
10%	90%

## Reading Material:

1. A review article identified by a senior academic staff member and other related literature.

Semester	1 or 2				
Course Code	CHEM 44832				
Course Name	Earth Resources and St	mart Materials			
Credit Value	2				
Compulsory/ Optional	Compulsory				
Pre- requisites		-			
Co- requisites	-				
Hourly Breakdown	Theory	Theory Practical Independent Learning			
	30	-	70		

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

- describe and apply the processing and utilization of various materials, minerals and earth resources
- describe different types of smart materials and their applications
- analyze critically regarding the applications and development of physical and chemical proceeding methods of nanomaterials

#### Course Content:

#### Earth Resources and Metallurgy (15 h)

Chemistry and identification of earth resources, petroleum crude oils, coal, natural gases, and minerals. Physicochemical properties and uses of petroleum crude oils, coal, natural gases, minerals and their commercial values. Mineral sands, titanium industry, appetite, graphite, quartz and silica. Minerals and material processing technology such as magnetic, electrical, gravitational and floatation techniques, pyrometallurgy, hydrometallurgy, electrometallurgy, alloys and steel, Ellingham diagrams, phase diagrams and related chemical properties, testing methods for metals and alloys.

#### Smart Materials (15 h)

Structure, properties, characterization and applications of fullerenes, nanotubes, graphene and its oxides, zeolites, silicone and liquid crystals. Introduction to nanotechnology. Nanomaterials structures, properties, preparation, characterization and applications.

**Teaching/ Learning Methods:** A combination of lectures and tutorials (supporting materials will be provided via CAL)

#### **Assessment Strategy:**

Continuous assessment and end of semester examination.

	Continuous Assessment	Final Assessment		
Details	20%		80%	
	Quizzes/ Assignments	Theory	Practical	Other
	20	80	-	-

- 1. Kent, J. A., (2003) Riegel's Handbook of Industrial Chemistry, Springer.
- 2. Marcaccio, M., Paolucci, F.,(2014) *Making and Exploiting Fullerenes, Graphene, and Carbon Nanotubes*, Springer.
- 3. Collings, P.J., (2000) *Liquid Crystals*, Princeton University press.
- 4. Lee, J.D. (2008), Concise Inorganic Chemistry, Blackwell.
- 5. Barry A. Wills., (2015) *Mineral Processing Technology*, 8th Edition, Pergamon Press.
- 6. Burkin, A.R., (2001) *Chemical Hydrometallurgy: Theory and Principles*, Imperial College Press.
- 7. Pradeep, T., (2012) *A textbook of Nanoscience and Nanotechnology*, Tata McGraw Hill Education Private Limited.
- 8. Murty,B.S., Shankar, P., Raj, B., Rath, B.B., Murday, J., (2013) *Textbook of Nanoscience and Nanotechnology*, Springer Universities Press.

## **University Level 4**

Semester	1 or 2			
Course Code	CHEM 44843			
Course Name	Advanced Biochemistr	y II		
Credit Value	3			
Compulsory/ Optional	Compulsory			
Pre- requisites		-		
Co- requisites		<del>-</del>		
Hourly Breakdown	Theory Practical Independent Learning			
	45	-	105	

## Course Aim/ Intended Learning Outcomes:

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

- describe advance techniques of gene manipulation and apply techniques to manipulate organisms and their products for human benefit
- describe the concepts of natural and acquired immunity and their roles and interaction in immune responses
- discuss processes involved in drug leads discovery, in modern -day rational drug design and development
- discuss the importance of biotechnology in drug industry

#### **Course Content:**

#### Gene technology (20 h)

Cloning genes in *E.coli*, and in higher organisms, various gene transfer methods, various strategies of isolating genes, gene sequencing, mutagenesis, analysis of gene structure and function, over production of proteins in *E. coil* and in higher organisms. PCR and its applications, molecular probes, markers and their uses, fingerprinting of genomes.

Impact of gene technology, disease diagnosis, human gene therapy, valuable products from cell culture. Various strategies of generating transgenic organisms for crop and livestock

improvement, metabolic engineering, fermentation methods, biofertilisers, biopesticides, industrial uses of enzymes, protein engineering, biosensors, biomass energy, biogas and biodiesel, biosafety, hazards and ethics, intellectual property rights and protection.

#### Immunology (10 h)

Cells and organs of the immune system, Innate vs. acquired immunity antigens, antibody structure and the generation of B-cell diversity, antigen-antibody reactions, monoclonal antibodies antibody genes. Major histocompatibility complex, T-cell mediated immunity B- cell mediated immunity. Cytokines, the complement system cell-mediated effector responses (CTL, NK, DH), immune responses to infection vaccines, hypersensitive reactions (immunopathologies) AIDS and other immuno-deficiencies autoimmunity transplantation, cancer and the immune system.

#### Pharmaceutical chemistry (15 h)

Drug-receptor theories, drug development, lead discovery, lead optimization, forces related to drug binding, chiral drugs, QSAR, Hansch equation and its uses, drugs targeting nucleic acids and enzymes, antibacterial drugs, cholinergics and anticholinergics, acetylcholinesterases, NSAIDS and opium analgesics, mechanisms

of development of drug resistance, drug synergism, pharmacogenomics, biotechnology based drugs, antisense oligonucleotides and RNA interference, as therapeutic agents, drug absorption and distribution, pharmacokinetics, metabolism of drugs, drug excretion phase, target based rational drug discovery. Plants as sources of drugs, traditional medicines and aromatherapy.

**Teaching/ Learning Methods:** A combination of lectures and tutorials (supporting materials will be provided via CAL)

## Assessment Strategy:

Continuous assessment and end of semester examination.

	Continuous Assessment	Final Assessment		
Details	20%		80%	
2 Cums	Quizzes/ Assignments	Theory	Practical	Other
	20	80	-	-

- 1. Brown, T. A., (2011) Introduction to Genetics: A Molecular Approach, Garland Science.
- 2. Old, R. W., Primrose, S. B., (1989) *Principles of Gene Manipulation, an Introduction to Genetic Engineering*, Blackwell.
- 3. Smith J. E., (2004) *Biotechnology*, Cambridge university press
- 4. Johnstone, A. P., Turner, M. W., (1997) Immunochemistry 2: A Practical Approach, Oxford.
- 5. Patrick, G. L., (2017), An Introduction to Medicinal Chemistry, Oxford University Press.

Semester	1 or 2				
Course Code	CHEM 44854				
Course Name	Advanced Environment	tal Chemistry			
Credit Value	4				
Compulsory/ Optional	Compulsory				
Pre- requisites	<u>-</u>				
Co- requisites		-			
Hourly Breakdown	Theory	Theory Practical Independent Learning			
	60	-	140		

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

- apply chemical principles of various fundamental environmental phenomena and processes in soil, water, and air
- apply basic concepts of chemical thermodynamics, kinetics, and photochemistry to analyze chemical processes involved in different environmental problems
- develop an awareness of the possible effects of chemicals on the environment
- describe the interconnections between different sectors of the environment (soil, water, atmosphere)
- describe and identify the effect of human activities on the natural chemical processes

#### **Course Content:**

## Aquatic Chemistry (10 h)

Characterization of different water bodies; physical, chemical and biochemical properties of water in different conditions. Interactions of water and air, interactions of water and soil, chemical reactions in water, aquatic microbial chemistry, transformation of different elements, colloids and sedimentation, water quality parameters, water pollution and water quality assessments, water purification techniques.

## Atmospheric Chemistry (10 h)

Physical characteristics of the atmosphere; temperature and pressure profiles. Chemistry of stratosphere; Chapman mechanism, polar ozone depletion. Chemistry of troposphere; one -box model, organic and inorganic pollutants, chemical and photochemical reactions, effect of air pollutants on health and ecosystem, control strategies. Sources and transformations of tropospheric and stratospheric aerosols and particulate matter.

#### Soil Chemistry (10 h)

Soil formation, soil minerals and organic matter, profile, texture, acidity, alkalinity and salinity of soil, base saturation and cation exchange capacity, nutrients and their availability, soil air, soil water, natural and anthropogenic terrestrial pollution.

#### Chemical Ecology (10 h)

Chemical interactions in eco-systems; semiochemicals and their classification. Inter species communications; pheromones, intra species communications. Allelochemicals; host —plant compounds, plant and animal defense compounds. Stereochemistry-bioactivity relationship; methodologies in chemical ecology, isolation of volatiles, electrophysiological assay, detection of biological activity, GC-EAD and GC-MS, semiochemicals as a pest control agent.

#### Waste Management (10 h)

Nature, sources and classification of waste, waste in the atmosphere, hydrosphere and geosphere. Reduction, treatment and disposal of waste. Waste minimization and cleaner production.

#### Impact of Agrochemicals in the Environment (10 h)

Classification, toxicity, mode of action, synthesis, bio pesticides, fate of pesticides in the environment, pesticide risk assessments, best management practices.

**Teaching/ Learning Methods:** A combination of lectures and tutorials (supporting materials will be provided via CAL)

## Assessment Strategy:

Continuous assessment and end of semester examination.

	Continuous Assessment	Final Assessment		
Details	20%		80%	
	Quizzes/ Assignments	Theory	Practical	Other
	20	80	-	-

- 1. Bunce, N., (1998) Environmental Chemistry, Wuerz.
- 2. Williams, I., (1999) Environmental Chemistry, A Modular Approach, John Wiley.
- 3. Evangelou, V. P., (1998) *Environmental Soil & Water Chemistry. Principle and Applications*, John Wiley.
- 4. Harrison, R. M., (1999) *Understanding our Environment. An introduction to Environmental Chemistry and Pollution*, RSC.
- 5. Hassal, K. A., (1990) The Biochemistry and Uses of Pesticides, Macmillian.
- 6. Green, M. B., Hartley, G. S., West, T. F., (1987) *Chemicals for Crop Improvement and Pest Management*, Pregaman.
- 7. Coping, L. G., Hewitt, H. G., (1998) Chemistry and Mode of Action of Crop Protection Agents, RCS
- 8. Barbara J. Finlayson-Pitts (1999) *Chemistry of the Upper and Lower Atmosphere*, Academic Press.

Semester	1 or 2				
Course Code	CHEM 44863				
Course Name	Advanced Inorganic Ch	Advanced Inorganic Chemistry II			
Credit Value	3	3			
Compulsory/ Optional	Compulsory				
Pre- requisites		-			
Co- requisites		-			
Hourly Breakdown	Theory Practical Independent Learning				
	45	-	105		

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

- explain the theories of NMR, ESR, NQR and Mossbauer spectroscopy
- propose structures of organic, inorganic and organometallic compounds based on NMR, ESR, NQR and Mossbauer spectroscopy data
- explain the mechanics of solid state devices by applying the knowledge of solid state reactions and physical properties of solids
- describe metals and their functions in biological systems
- postulate structures of cluster compounds and thereby predict properties of such compounds

#### **Course Content:**

#### Spectroscopic Methods (15 h)

Principles of NMR (<sup>19</sup>F, <sup>31</sup>P, <sup>13</sup>C, <sup>14</sup>N and <sup>11</sup>B), ESR, pulse NMR, spin lattice relaxation time, variable temperature NMR, NQR, Mossbaur spectroscopic techniques and their applications in structural elucidation of inorganic and organometallic compounds.

#### Solid State Chemistry (15 h)

Crystal structures of binary compounds, crystals defects, free electron model, Fermi-Dirac distribution, band theory. Electrical transport in solids; conductivity, metals, semiconductors and insulators and their applications, semiconductor junctions, diodes and transistors, superconductivity. Thermal and magnetic properties, solid state reactions, techniques used in solid state synthesis, conducting organic polymers.

#### Chemistry of Metal Clusters (5 h)

Quadruple bond, binuclear to polynuclear metal clusters, structure elucidation methods.

## Bioinorganic Chemistry (10 h)

Metals in biological systems, metalloenzymes, dioxygen carriers, biological redox reactions, distribution and functions of metals, metal induced toxicity and chelation therapy, environmental bioinorganic chemistry.

**Teaching/ Learning Methods:** A combination of lectures and tutorials (supporting materials will be provided via CAL)

#### Assessment Strategy:

Continuous assessment and end of semester examination.

Percentage given for each subcomponent indicates the percent contribution to the final marks

	Continuous Assessment	Final Assessment		
Details	20%		80%	
Bouns	Quizzes/ Assignments	Theory	Practical	Other
	20	80	-	-

- 1. Friebolin, H., (2010) Basic One and Two Dimension NMR Spectroscopy, Methu.
- 2. Bancroft, G. N., (1973) Mossbauer Spectroscopy, McGraw Hill.
- 3. West, A. R., (2014), Solid State Chemistry and its Applications, John Wiley & Sons Ltd.
- 4. Sharpe, A.G., (2002) *Inorganic Chemistry*, Pearson.
- 5. Cotton, F.A., Wilkinson, G., Murillo, C. A, Bochmann, M; (2007), *Advanced Inorganic Chemistry*, New York, John Wiley.
- 6. Kaim, W., Schwerderski, B., (2013) *Bioinorganic Chemistry-Inorganic Elements in the Chemistry of Life*, John Wiley.
- 7. Liyanage, J. A., (2014), Life and Metals, Monograph No 19, College of Chemical Sciences.
- 8. Liyanage, J. A., (2013), *Hard & Soft Acids & Bases, Monograph No 16*, College of Chemical Sciences.

Semester	1 or 2				
Course Code	CHEM 44874				
Course Name	Advanced Organic Che	mistry II			
Credit Value	4				
Compulsory/ Optional	Compulsory				
Pre- requisites	-				
Co- requisites		-			
Hourly Breakdown	Theory	Theory Practical Independent Learning			
	60	-	140		

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

- explain the reactivity and major synthetic pathways of heterocyclic compounds
- identify different stereochemical representations and describe the reactions and synthesis of mono and disaccharides
- explain various molecular recognition mechanisms in different functional processes
- explain the interactions between electromagnetic radiations and matter and mechanisms that control these interactions
- explain the formation of products in pericyclic reactions by frontier orbital, aromatic concept and conservation of orbital symmetry theories.
- describe the contemporary use of natural products
- describe biosynthetic pathways of terpenes, steroids and alkaloids

#### Course Content:

#### Advanced Heterocyclic Compounds (10 h)

Reactions and synthesis of five membered heterocyclic compounds with one hetero atoms and two heteroatoms; electrophilic reactions on hetero atom (protonation, nitration, sulfonation, amination, halogenation, acylation), electrophilic substitution reactions on carbon atom (nitration, sulfonation, halogenation), reactions with nucleophiles (hydride transfer, displacement of good leaving group), metalation and reactions with electrophiles, Palladium catalyzed coupling reactions, radical reactions, carbonyl condensation type reactions; Knorr synthesis, Paar-Knorr synthesis. Cyclo additions: nitrene insertion; pyridines, pyridones, alkylpyridines, quaternary pyridinium salts, pyridine N-oxides, quinolenes, isoqunolenes,pyrrole, pyrylium ions, pyrones, diazenes, indoles, thiophenes, oxithiophenes, furans, 1,3-azoles.

## Carbohydrates (10 h)

Stereochemistry of carbohydrates; Fischer projections, Haworth formulae, D & L and R/S nomenclature. Conformational analysis; anomeric and reverse anomeric effects, preferred conformations of pyranoses. Reactions at anomeric center; formation and hydrolysis of glycosides. Reactions of hydroxyl groups; ethers, esters, blocking groups. Reaction sat non-anomeric carbon atoms; nucleophilic displacement of leaving groups, ring opening reactions, amino, thio and deoxy sugars. Synthesis of monosaccharides and disaccharides, structure determination of carbohydrates.

#### Supramolecular Chemistry (10 h)

Concepts and language of supramolecular chemistry. Non-covalent bonds involved in supramolecular complexes; hydrogen bonding, electrostatic forces,  $\pi$ - $\pi$  stacking interactions, Van der Waals bonds,

hydrophobic /solvophobic forces. Introduction to molecular recognition; recognition, information, complementarity, molecular receptors and substrates. Supramolecular reactivity and catalysis and transport processes and carrier design(ionophores), cations, anions and neutral molecules binding hosts (crown ethers, cryptands, spherands) and spherical and tetrahedral recognition shown by these hosts, coreceptor molecules and multiple recognition (dinuclear and polynuclear metal ion cryptates, recognition of molecular length by ditopic co receptors, heterotopic co receptors and metallo receptors).

## Concerted Reactions and Organic Photochemistry (15 h)

Characteristic features of concerted reactions, Woodward–Hoffmann rules, pericyclic reactions and their classifications as electrocyclic, sigma tropic and cycloaddition reactions, theoretical predictions of occurrence and stereochemical outcome of pericyclic reaction (under thermal and photochemical conditions) using frontier orbital, aromatic concept and conservation of orbital symmetry theories. Photodissociation; photodissociation of carbonyl compounds, photochemical chlorination of methane. Fundamental photochemistry of simple carbonyl compounds and enones; excited states of the carbonyl group, intermolecular and intramolecular hydrogen abstraction, photochemical additions to alkenes and alkynes with and without sensitizers-oxetane formation. Photochemistry of simple olefins, polyenes and aromatic compounds; geometrical isomerisation, cycloaddition of non-conjugated alkenes, Zimmerman rearrangement, photoisomerisation of benzavalene, fulvalene, Dewar benzene and prismane intermediates. Applications of photochemistry; photochromism, simple, photochemistry of vision.

#### Natural Products (15 h)

Link between primary and secondary metabolites, Diversity and classification: Terpenes, steroids, alkaloids, polyketides, phenyl propanoids, flavonoids etc. Synthesis and uses of commercially important monotepenes, sesquiterpenes, triterpenoids, triterpenoids, biological function of triterpenoids and steroids. Steroids; nomenclature and medicinal uses of bile acids, plant sterols, cardiac glycosides, vitamins, steroid hormones.

Biosynthesis of major classes of natural products; chemistry and interconnectivity of biosynthetic pathways of key intermediates, monoterpenes via mevalonic acid pathway, biosynthesis of di and tri terpenoids, biosynthesis of squalene via cyclopropane, elucidation of biosynthetic pathways; feeding experiments, biosynthesis of bioactive compounds via polyketide pathway, biosynthesis of selected examples of steroids

Alkaloids; Major reactions in biosynthesis (oxidative deamination, decarboxylation, transamination, reductive amination etc.), alkaloid methylation patterns, origin of heterocyclic rings from specific amino acids, biosynthesis and pharmacognostic studies of pyridine, piperidine, tropane, imidazole, isoquinoline, quinoline, indole, purine, steroidal diterpene and phenethylamine groups.

**Teaching/ Learning Methods:** A combination of lectures and tutorials (supporting materials will be provided via CAL)

## Assessment Strategy:

Continuous assessment and end of semester examination.

	Continuous Assessment	Final Assessment		
Details	20%	80%		
Details	Quizzes/ Assignments	Theory	Practical	Other
	20	80	-	-

- 1. Murphy, P. (2002) *Heterocyclic Chemistry; Series: Tutorial Chemistry Texts*. M. Sainsbury, University of Bath. Chem. Educator.
- 2. Robyt, J.F., (1998) Essentials of Carbohydrate Chemistry, Springer.

- 3. Steed J.W., Atwood J.L., (2000) Supramolecular Chemistry, John Wiley & Sons.
- 4. Lehn J.M., (1995) Supramolecular Chemistry, Concepts and Perspectives, VCH.
- 5. Nicholas J. T., (1991) Modern Molecular Photochemistry, University Science Books.
- 6. Coyle, J. D., (1986) Introduction to Organic Photochemistry, John Wiley.
- 7. Dewick, P. M., (2000) Medicinal Natural Products: A Biosynthetic Approach, John Wiley.
- 8. Mann J, (1995) Chemical Aspects of Biosynthesis, Oxford Chemistry Primers.
- 9. Bohl, M. and Duax, W. L., (2000) *Molecular Structure and Biological Activity of Steroids*, CRC Press.

Semester	1 or 2					
Course Code	CHEM 44884					
Course Name	Advanced Physical Che	Advanced Physical Chemistry II				
Credit Value	4	4				
Compulsory/ Optional	Compulsory					
Pre- requisites		-				
Co- requisites	-					
Hourly Breakdown	Theory Practical Independent Learnin					
	60	-	140			

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

- use the knowledge in electrochemistry for evaluation of equilibrium and non-equilibrium electrochemical processes and apply the knowledge on industries based on electrochemistry phenomena
- apply the fundamentals of rotational, vibrational and Raman spectroscopy to diatomic and poly atomic molecules and calculate basic structural parameters
- apply the basic principles of photochemistry and explain examples of the effects of photochemistry in nature and in various industrial applications.
- visualize molecular structure and build optimized molecular models with computers
- describe the physical structure of solid surfaces and the behavior of gases on adsorption at surfaces
- demonstrate knowledge of quantitative and qualitative surface analysis techniques
- explain how the partition function is determined for a thermodynamic system and how it can be used to determine thermodynamic properties

#### **Course Content:**

#### Electrochemistry (15 h)

Ion—solvent interaction; models for ion—solvent interactions, solvation enthalpy, entropy and free energy. Ion-ion interaction; Debye-Hückel theory for mean activity coefficients of electrolytes. Electro-capillary phenomenon and model for the charge distribution at the electrode—electrolyte interface. Kinetics of electrode reactions; Butler—Volmer formalism. Tafel relationship. Corrosion of metals; thermodynamics and kinetics of corrosion, Pourbaix and Evans diagrams, corrosion current and corrosion potential, corrosion control methods. Electro-technology; electroplating and other related techniques.

#### Molecular Spectroscopy (15 h)

Rotational spectroscopy; rigid rotor, rotational spectra of diatomic molecules, rotation levels of polyatomic molecules: spherical, symmetric, and asymmetric tops, spectral line widths and intensities. Vibrational spectroscopy; vibration of diatomic molecules. harmonic and anharmonic oscillator, fundamentals, overtones, combination bands, hot bands, vibrational-rotational couplings, vibration of polyatomic molecules. Vibrational and rotational fine structure, Franck—Condon principle Raman spectroscopy; rotational and vibrational Raman spectra.

#### Photochemistry (10 h)

Basic principles of photochemistry; photophysical processes and photodissociation, absorption and emission of radiation; selection rules of electronic excitation, Jablonski diagram, singlet and triplet states, fluorescence and phosphorescence, intersystem crossing, radiative and non-radiative decays;

kinetics of photophysical processes: quantum yield, lifetime, quenching, Stern-Volmer plots; lasers, chemiluminescence, vision and photoimaging.

## Surface Chemistry (10 h)

Adsorption & desorption at surfaces, adsorption isotherms and desorption kinetics, Surface analysis; photoelectron spectroscopy, Auger electron spectroscopy, scanning tunneling microscopy, atomic force microscopy, secondary ion mass spectroscopy, laser induced desorption, electron energy loss spectroscopy, low energy X-ray diffraction, reflectance IR spectroscopy. Heterogeneous catalysis; Langmuir-Hinshelwood mechanism, Ely-Rideal mechanism, supported catalysts.

## Statistical Thermodynamics (10 h)

Quantum states, Maxwell-Boltzmann, Bose-Einstein and Fermi- Dirac statistics, statistical ensembles: canonical, microcanonical and grandcanonical ensembles, partition functions: translational, rotational, vibrational and electronic partition functions of gases, Relation of state functions to the partition function. Boltzmann distribution law for non-interacting particles, statistical thermodynamics of ideal monoatomic, diatomic and polyatomic gases

**Teaching/ Learning Methods:** A combination of lectures and tutorials (supporting materials will be provided via CAL)

## Assessment Strategy:

Continuous assessment and end of semester examination

	Continuous Assessment	Final Assessment		
Details	20%	80%		
Details	Quizzes/ Assignments	Theory	Practical	Other
	20	80	-	-

- 1. Donald, T.S., Andrzej, S., Julian, L.R. Jr., (2015) *Electrochemistry for Chemists*, John Wiley.
- 2. Eliezer, G., (1993) *Electrode Kinetics for Chemists, Chemical Engineers and Materials Scientists*, Wiley-VCH.
- 3. Nestor, P., (2016), Electrochemistry & Corrosion, Springer.
- 4. Bockris, J. O. M. and Reddy, A. K. N. (2002), *Modern Electrochemistry*, Vol 1 and 2, Springer-Verlag.
- 5. Pletcher, D. (2019) A First Course in Electrode Processes, RSC.
- 6. Birdi, K.S., (2015) Handbook of Surface and Colloid Chemistry, CRC Press.
- 7. Banwell, C. N., (2017) Fundamentals of Molecular Spectroscopy, McGraw Hill.
- 8. Hollas, J. M., (2013) High Resolution Spectroscopy, Butterworth-Heinemann.
- 9. Hollas, J. M., (2004) *Modern Spectroscopy*, John Wiley.
- 10. Wayne, C. E., Wayne, R. P., (1996) Photochemistry, Oxford.
- 11. Atkins, P. W., (2018) Physical Chemistry, Oxford.
- 12. Levine, I. N., (2011) Physical Chemistry, McGraw-Hill.

Semester	1 or 2	1 or 2				
Course Code	CHEM 44893	CHEM 44893				
Course Name	Chemical Engineering Chemistry	Chemical Engineering and Management Concepts in Industrial Chemistry				
Credit Value	3	3				
Compulsory/ Optional	Compulsory	Compulsory				
Pre-requisites	-					
Co-requisites	-					
Hourly Breakdown	Theory	Theory Practical Independent Learning				
	45	-	105			

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

- explain and analyze different quality management frameworks
- aware of available techniques, software and web-resources for cheminformatics.
- demonstrate and apply the knowledge of chemical engineering concepts and management systems in industrial chemistry
- demonstrate and apply the knowledge of chemical engineering concepts and management systems in industrial chemistry

#### **Course Content:**

## Quality and Laboratory Management (20 h)

Introduction: Importance of quality in the management process. Concepts of quality management. Quality dimensions of goods and services. Quality management evolution and works of quality founders. Quality policy and quality organizations: International quality organizations. International, regional and national standardization. System of assessment of quality conformity.

Management systems and quality management principles for excellence: Quality management systems. Quality control methods. Quality audit and certification of management systems. Sustainable development. Environment management systems. Occupational health and safety management system. Total quality management.

Statutory regulations governing health and safety, laboratory design and accreditation, hazard monitoring and waste minimization and chemical disposal. ISO/IEC 17025:2017

#### **Introduction to Cheminformatics (5 h)**

History and evolution of Cheminformatics, Chemical representation, Sequence, 2D, 3D structure, Types of chemical representation

Chemical databases, combinatorial chemistry, combinatorial library design, Application of cheminformatics.

#### Fundamentals of Chemical and Process Engineering (20 h)

Basic principles in chemical and process engineering

Unit operations: Mixing, drying, adsorption, separation, filtration, distillation etc.

Process flow sheeting: Types of flow diagrams

Material and energy balances: Non-reacting and reacting systems with single and multiple reactions Reduction and enlargement: Size separation, processes and equipment for size reduction and enlargement

Introduction to fluid mechanics

Heat transfer: Modes of heat transfer and calculations

Mass transfer: Calculations and different mass transfer operations

Introduction of chemical reactors: Different reactor types, basic calculations and reactor selection

**Teaching/ Learning Methods:** A combination of lectures and tutorials (supporting materials will be provided via CAL)

## Assessment Strategy:

Continuous assessment and end of semester examination.

	Continuous Assessment	Final Assessment		
Details	ails		80%	
2 Culto	Quizzes/ Assignments	Theory	Practical	Other
	20	80	-	-

- 1. Dale, B. G. (2003) Managing Quality. Oxford: Blackwell Publishing.
- 2. Goetsch D. L., Davis S. B. (2003) Quality *Management. Introduction to TQM for Production, Processing and Services*. New Jersey: Prentice Hall.
- 3. Harmening D.M., (2020) Laboratory Management: Principles and Processes. Prentice Hall.
- 4. Andrew R. Leach & Valerie J.Gillet, (2007) *An Introduction to Cheminformatics*, Springer Publication.
- 5. Reklaitis G. V., (1983) Introduction to Material and Energy Balances, Wiley Publication.
- 6. Simons S. J. R., (2019) Concepts of Chemical Engineering for Chemists, RSC publishing.
- 7. Cengel Y., Ghajar A., J., (2019) *Heat and Mass Transfer: Fundamentals and Applications*, Mc Grow Hill Publications.
- 8. Richardson, J.F., Harker, J.H., Backhurst, J.R., (2019)*Coulson and Richardson's Chemical Engineering Volume 2*, Elsevier Publications.

Semester	1 or 2					
Course Code	CHEM 44902					
Course Name	Food Chemistry	Food Chemistry				
Credit Value	2					
Compulsory/ Optional	Compulsory					
Pre- requisites		-				
Co- requisites		-				
Hourly Breakdown	Theory	Practical	Independent Learning			
	30	-	70			

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

- describe the structure and physiochemical properties of major food components and their use in the food
- explain biochemical changes occurring in raw foods
- describe effect of processing on food colors, flavors, odors and nutritional quality
- apply knowledge and understanding of technology behind processing of food products
- apply the methods and skills used in food analysis

#### Course Content:

Food carbohydrates, lipids and protein; their structure, occurrence, physiochemical properties and application in food industry; Biochemical changes occur in raw foods, meat, fish, fruit, vegetables, cereal and milk etc; Biochemistry of food spoilage, browning, rancidity, staling etc; Food additives, preservatives, antimicrobials, sweeteners and others; Food colors, natural and artificial food colors, effect of processing on food colors; Flavors and odor, chemical basis of taste, sweet, salty, bitter and sour compounds, flavors and odors in common foods, effect of food processing on flavors and odors; Food contaminants, natural toxicants, AOAC methods in food analysis, genetically modified (GM) foods, food laws, safety and regulations.

**Teaching/ Learning Methods:** A combination of lectures and tutorials (supporting materials will be provided via CAL)

## Assessment Strategy:

Continuous assessment and end of semester examination.

	Continuous Assessment	Final Assessment		
Details	Details 20%		20% 80%	
	Quizzes/ Assignments 20	Theory 80	Practical -	Other -

- 1. Coultate, T.P., (1996), Food: The Chemistry of its Components, RSC, Cambridge.
- 2. Ramaswarmy, H., Marcotte M., (2006), *Food Processing Principles and Applications*, Taylor and Francis Publishers.
- 3. Richardson T., Finley J. W., (1997), *Chemical Changes in Food during Processing*, CBS Publishers.
- 4. Vaclavik V.A., (1998), Essentials of Food Science, Chapman and Hall.

Semester	1 or 2					
Course Code	CHEM 44912					
Course Name	Polymer Chemistry	Polymer Chemistry				
Credit Value	2	2				
Compulsory/ Optional	Compulsory					
Pre-requisites		-				
Co-requisites		-				
Hourly Breakdown	Theory	Theory Practical Independent Learning				
	30	-	70			

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

- describe polymer synthesis and characterization methods
- predict the properties of polymers through structure-property relationships
- summarize industrially important polymers, their structures, polymerization processes and applications
- explain the environmental effects caused by polymers and methods to minimize such effects
- apply the knowledge in polymer-related product manufacturing

#### **Course Content:**

Various classifications of polymers, polymer synthesis, characterization and properties, Industrially important polymers: structure, preparation, characterization and properties, structure-property relationships, Environmental effects of polymers: degradation and stabilization
Introduction to natural and synthetic lattices, stabilization of lattices, preservation of natural rubber (NR) latex, preparation methods of concentrated NR latex, characterization of NR latex, deproteinized NR latex, additives used in latex processing, latex compounding and vulcanization methods
Polymer- related industries: dry rubber- based and latex-based industries, paints and surface coatings, plastics industry

**Teaching/ Learning Methods:** A combination of lectures and tutorials (supporting materials will be provided via CAL)

#### **Assessment Strategy:**

Continuous assessment and end of semester examination.

	Continuous Assessment	Final Assessment		
Details	20%	80%		
2 Coming	Quizzes/ Assignments	Theory	Practical	Other
	20	80	-	-

- 1. Ravve, A., (1995) Principles of Polymer Chemistry, Plenum.
- 2. Billmeyer, F. W., (1984) Textbook of Polymer Science, John Wiley.
- 3. Seymour, R.D. and Carraher Jr. E.R., (1992) *Polymer Chemistry; An Introduction*, Marcel Dekker Inc.
- 4. Young, R. J. and Lovell, P. A. (2011), Introduction to Polymer Chemistry, CRC Press.

Semester	1 and 2					
Course Code	CHEM 43928					
Course Name	Research Project- Diss	Research Project- Dissertation				
Credit Value	8	8				
Compulsory/ Optional	Compulsory					
Pre- requisites		-				
Co- requisites	-					
Hourly Breakdown	Theory Practical Independent Learning					
	-	360	40			

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

• plan and carryout a research project on chemistry according to the scientific methods, accumulate and analyze experimental data, interpret and report the results in a scientific manner and to present and defend findings to the scientific community

## Course Content:

A research project in chemistry or in a related area of chemistry

**Teaching/Learning Methods:** Literature survey, laboratory and/ or field work, data analysis and interpretation, dissertation, presentations.

## **Assessment Strategy:**

Continuous assessments; dissertation, progress reports, presentations, *viva - voce* examination.

	Evaluation by Mentor	Final Assessment		
Details		50%		
2 000015		Thesis	<i>viva – voce</i> examination.	
	50%	30	20	