Maulana Abul Kalam Azad University of Technology, West Bengal

Course: M.Sc. in Applied Chemistry
Duration: 2 Years; **Level**: Post graduation; **Type**: Degree

SEMESTER - I

Sl. No.	Paper code	Course name	Course type	Marks	Hours/credit			
					L	T	P	C
1.	MSAC101	Organic Chemistry I	CC **(Theory)**	100	3	0	0	3
2.	MSAC102	Advanced Inorganic Chemistry	CC **(Theory)**	100	3	0	0	3
3.	MSAC103	Advanced Physical Chemistry	CC **(Theory)**	100	3	0	0	3
4.	MSAC104	Analytical Techniques	CC **(Theory)**	100	3	0	0	3
5.	MSAC105	Numerical Methods in Computational Chemistry	CC **(Theory)**	100	3	0	0	3
6.	MSAC191	Lab Techniques for Quantitative and Qualitative Analysis	CC **(Practical)**	100	0	0	6	3
7.	MSAC192	Computer Programming –I	CC **(Practical)**	100	0	0	6	3
8.	MSAC193	Computer aided Stereo-chemical Analysis of Complex Chemical Reaction	CC **(Practical)**	100	0	0	4	2
9.	MSAC194	Project-I	SEC **(Sessional)**	100	0	0	4	2
10.	MSAC181	Audit Course	SEC **(Sessional)**	-	-	-	-	-
	Total			**900**	**25**			

SEMESTER - II

Sl. No.	Paper code	Course name	Course type	Marks	Credit			
					L	T	P	C
1.	MSAC201	Quantum Chemistry	CC **(Theory)**	100	3	0	0	3
2.	MSAC202	Statistical Mechanics	CC **(Theory)**	100	3	0	0	3
3.	MSAC203	Organic Chemistry II	CC **(Theory)**	100	3	0	0	3
4.	MSAC204	Nano science and technology	IDC **(Theory)**	100	3	0	0	3
5.	MSAC205	Applications of Artificial Intelligence and Machine Learning in Chemistry	SEC **(Theory)**	100	2	0	0	2
6.	MSAC206	Natural Products and Medicinal Chemistry	DSE **(Theory)**	100	3	0	0	3
7.	MSAC291	Computational Methods in Chemistry	CC **(Practical)**	100	0	0	6	3
8.	MSAC292	Advanced Chemistry Laboratory	CC **(Practical)**	100	0	0	6	3
9.	MSAC293	Project-II	SEC **(Sessional)**	100	0	0	6	3
	Total			**900**	**26**			

SEMESTER - III

Sl. No.	Paper code	Course name	Course type	Marks	Credit			
					L	T	P	C
1.	MSAC301	Bioorganic, Supramolecular and Green Chemistry	CC **(Theory)**	100	3	0	0	3
2.	MSAC302	Biochemistry & Bioinorganic Chemistry	DSE **(Theory)**	100	3	0	0	3
3.	MSAC303	Research Methodology	CF **(Theory)**	100	3	0	0	3
4.	MSAC304(A-D)	Elective I	EF **(Theory)**	100	3	0	0	3
5.	MSAC305(A-D)	Elective II	EF **(Theory)**	100	3	0	0	3
6.	MSAC391	Computer Programming–II	CC **(Practical)**	100	0	0	4	2
7.	MSAC392	Preparation of Complex Materials and their Characterization by Physiochemical Techniques	CC **(Practical)**	100	0	0	6	3
8.	MSAC393	Spectroscopic Analysis Lab	CC **(Practical)**	100	0	0	6	3
9.	MSAC394	Project-III	SEC **(Sessional)**	100	0	0	6	3

	Total		**900**	**26**

SEMESTER - IV

Sl. No.	Paper code	Course name	Course type	Marks	Credit			
					L	**T**	**P**	**C**
1.	MSAC401(A-D)	Elective III	EF **(Theory)**	100	3	0	0	3
2.	MSAC491	Industrial Exposure	VAC **(Sessional)**	100	0	0	4	2
3.	MSAC492	Project-IV (Dissertation & Viva voce)	CC **(Sessional)**	100	12			
	Total			**300**	**17**			

CC: Core Course, **VAC:** Value Added Course, **SEC:** Skill Enhancement Course, **IDC:** Interdisciplinary Course, **DSE:** Discipline Specific Elective, **EF:** Elective Foundation, **CF:** Compulsory Foundation

Elective Basket:

Elective I basket	Elective II basket	Elective III basket
A. Photochemistry and spectroscopy	A. Colloids, surface chemistry, catalysis and solid state	A. Pharmaceutical Chemistry
B. Cheminformatics	B.Industrial Chemistry	B.Food Chemistry
C. Water and Wastewater Treatment	C.Sensor Development	C.Industrial Catalysis
D. Semiconductor devices	D.Solid Waste Management and Air Pollution	D.Industrial & Environmental Pollution Management and Industrial Process Safety

Program summary:

Semesters	Contact Hours/week	Marks	Program credit
I	35	900	25
II	35	900	26
III	37	900	26
IV	31	300	17
	Total	**3000**	**94**

Maulana Abul Kalam Azad University of Technology, West Bengal

Course: M.Sc. in Applied Chemistry
Duration: 2 Years; **Level**: Post graduation; **Type**: Degree

SEMESTER-I

Organic Chemistry-I

Paper code: MSAC101
(3 Credit) (100 Marks)

Course Objectives:

1. To write and assign reactive intermediates, stereochemistry of organic compounds.
2. To learn advanced knowledge of pericyclic and photochemical reactions.
3. To learn about the role and applications of oxidising and reducing agents in organic synthesis
4. To impart advanced knowledge regarding various rearrangement reactions for synthetic applications.

Module 1: Unit 1: Organic Reaction Mechanism and Introduction to Stereochemistry (6L)
Methods of determining reaction mechanisms (kinetic and non-kinetic methods): The Hammond postulate, reactivity vs selectivity principle, the Curtin-Hammett principle, microscopic reversibility, kinetic vs thermodynamic control. Isotope effects. Linear free energy relationships: Hammett and Taft parameters, Other Experimental techniques to determine reaction mechanisms: cross - over experiments, isotope scrambling. Concept of centre and plane of chirality, axial chirality and point groups. Conformational analysis of cyclohexane, cyclohexene, cyclohexanone, alkyl ketone effect, 2-halo ketone effect, allylic strains, decalin and their derivatives; Felkin-Anh, Cieplak models; Addition reactions to carbonyl compounds.

Module 2: Unit 2: Pericyclic reactions, Aromatcity, Polynuclear hydrocarbons and Applications (10L)
Study of frontier molecular orbital theory, aromatic transtionstate theory and the generalized Woodward – Hoffmann rule applied to cycloaddtions, electrocyclic reactions, sigmatropic rearrangements and chelotropic reactions, stereochemistry and regiochemistry of cycloaddtions. Secondary orbital interactions in [4+2] cycloadditionsIntramolecular Diels–Alder reactions. 1,3-dipolar cycloaddition reactions. Photochromism and thermochromism, Cope rearrangement, Claisen rearrangement, and ene-reaction.
Aromatcity, Polynuclear hydrocarbons and their applications.

Module 3: Unit 3: Reagents in organic synthesis (10L)
Oxidation: metal-based oxidants (Cr, Mn, Se, Os, Ag, Tl, Ru and Pb); non-metal-based oxidation: Swern oxidation, Moffat oxidation, Organic oxidants, Chemistry of hypervalent iodine based oxidants, CAN as oxidant.

Reduction: metal hydrides (B-H, Al-H, Zn-H, Sn-H, Si-H based reagents); hydrogenation; dissolving metal reductions; samarium iodide, Organic reductants.
Chemistry of organosilicon compounds, Synthetic uses of silyl ethers, silylenol ethers, alkene synthesis, alkynyl, vinyl, aryl, allyl and acyl silanes; Brook rearrangement, silicon Baeyer-Villiger rearrangement. Ionic hydrogenation, synthetic use of TMSCN, TMSNCO, TMSI, TMSNHCOMe, $TMSN_3$ etc.

Module 4: Unit4: Name reactions & Rearrangements reactions (10L)

General mechanistic considerations, nature of migration, migratory aptitude, nucleophilic, electrophilic and free radical rearrangements. Name reactions: Baylis – Hillman reaction, Shapiro reaction, Mitsunobu reaction, Julia olefination, McMurry reaction etc. Rearrangements reactions - Wagner-Meerwein, McLafferty, Demyanov, Benzil-benzilic acid, Favorskii, Fritsch-Buttenberg-Wiechell, Neber, Hofmann, Curtius, Beckmann, Schmidt, Lossen, Wolff, Baeyer-Villiger, Dienone-phenol, Pinacol, Stevens, Wittig, Chapman, Wallach, Orton, Bamberger, Pummerer and von Richter rearrangements.

Text Books:

1. March's *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 7th ed. 2013, Wiley
2. F. A. Carey and R. J. Sundberg: *Advanced Organic Chemistry (parts A and B)*, 5th Edition2008, Springer.
3. J. Clayden, N. Green, S. Warren and P. Wothers: *Organic Chemistry*, 2nd Edition. 2012, Oxford University Press

Refrence texts:

1. T H.Lowry and K.S.Richardson: *Mechanism and Theory in Organic Chemistry*, 3rd ed. 1997, Benjamin-Cummings Publishing Company.
2.F. A. Carroll: *Perspectives on structure and mechanism in organic chemistry*, Wiley, 2011 edition.
3. *Organic Stereochemistry* by P.S. Kalsi.
4. I. Flemming: *Molecular orbitals and organic chemical reactions*, student edition, 2009, Wiley.
5. J. McMurry, *Organic Chemistry*, Fifth Edition, 2000, Brooks/Cole .

Sl.No	Content of the course	Module No.	%age of questions	Course Outcomes (CO)	CO	PO
1.	Organic reaction mechanism and introduction to stereochemistry	Module-1/ Unit-1	20%	1. To be able to predict reaction intermediates, stereochemistry of organic compounds.	CO1	PO1
2.	Pericyclic reactions, aromaticity, polynuclear hydrocarbons and applications	Module-2/Unit-2	30%	2. To be able to address problems on pericyclic and photochemical reactions.	CO2	PO1
3.	Oxidising and reducing agents in organic synthesis	Module-3/Unit-3	30%	3. To be able to explore the role and applications of oxidising and reducing agents in organic synthesis.	CO3	PO1
4.	Rearrangement reactions	Module-4/Unit-4	20%	4. To impart advanced knowledge regarding various rearrangement reactions for synthetic applications.	CO4	PO1

Advanced Inorganic Chemistry

Paper code: MSAC102
(3 Credit) (100 Marks)

Course Objectives:

1. To effectively learn the fundamentals of the chemistry of the main group elements, and important real world applications of many of these species.
2. To learn the key concepts of inorganic chemistry related synthesis, reaction chemistry, structure and bonding.
3. To impart advanced knowledge regarding transition metal and inner transition metal chemistry.

Module 1: Unit 1: Main Group Elements **(10L)**

Main group elements and their compounds: Allotropy, synthesis, structure and bonding. Synthesis, Properties, Structure and Bonding of: Nitrogen, Phosphorous, Sulfur, Pseudohalogen, Interhalogen and Xenon Compounds, Borazines, Phosphazenes, Sulfur-Nitrogen compounds, Silicones, bonding and reactions in higher boranes, Wades rules and styx numbers, Carboranes, Metallocarboranes. Isolobal analogy, PSEPT theory, Capping principle.

Module 2: Unit 2: Reactions and structures **(10L)**

Polyhedral rearrangements, Fragmentation reactions, Isopoly & heteropoly acids & salts. Introduction, properties, structure, bonding, organometallic chemistry, synthesis and reactivity of organo lithium, beryllium, and magnesium compounds. Boron, aluminum, gallium, indium organyls, germanium, tin and lead organyls, multiple bonded compounds, cages, clusters.

Module 3: Unit 3: Coordination Chemistry **(12L)**

CFT and its limitations, LFT, MOT. Classification of ligands by donor atoms, stability, reactivity, bond types, geometry and coordination compounds. Kinetics and mechanism of reactions of transition metal complexes: substitution reactions, electron transfer redox processes, acid base and related processes. Electronic Spectra of transition metal complexes. Spectroscopic ground states, Orgel, Tanabe Sugano, Correlation diagram, Charge transfer spectra.

Module 4: Unit 4: Inner transition elements **(8L)**

Definition of magnetic properties. Curie and Curie-Weiss Law, Orbital and spin contribution to magnetic susceptibility, Magnetic exchange coupling, Spin cross over phenomena. Inner transition elements: spectral and magnetic properties, redox chemistry, analytical applications.

Text books:

1. Concise Inorganic Chemistry - J. D. Lee
2. Inorganic Chemistry - J. E. Huheey

Reference texts:

3. Inorganic Chemistry -Meissler & Tarr
4. Mechanism of Inorganic Reactions – Fred Basolo, Ralph G. Pearson

Sl. No	Content of the course	Module No.	%age of questions	Course Outcome (CO)	CO	PO
1	Main Group Elements	Module 1/Unit 1	25%	1. To effectively learn the fundamentals of the chemistry of the main group elements, and important real world applications of many of these species.	CO1	PO1
2	Reactions and structures	Module 2/Unit 2	25%	2.To learn the key concepts of inorganic chemistry related synthesis, reaction chemistry, structure and bonding.	CO2	PO1
3	Coordination Chemistry, Inner transition elements	Module 3/Unit 3, Module 4/Unit 4	50%	3.To impart advanced knowledge regarding transition metal and inner transition metal chemistry	CO3	PO1

Advanced Physical Chemistry

Paper code: MSAC103
(3 Credit) (100 Marks)

Course Objectives:

1. Effectively learn the group theory and its use for molecular term symbol.
2. Will be expertise to predict the reaction rate using computer softwere.
3. Will be able to treat ionic reaction probably.
4. Information regarding thermodynamic properties of different systems which may be applied to understand the equilibrium conditions of chemical reactions.

Module 1: Unit 1: Symmetry & Group Theory **(10L)**

Symmetry elements & operations; group, subgroup, class, point groups, group multiplication tables for cyclic and non-cyclic groups; matrix representations of symmetry operations and their characters,reducible representations, irreducible representations and great orthogonality theorem (no derivation), construction of character tables; application of group theory.

Module 2: Unit 2: Thermodynamics **(10L)**

Laws of Thermodynamics, General condition of Equilibrium, Entropy, Partial molar quantities, their significance. Thermodynamic properties of gases with special reference to real gas in pure state and in mixture. Thermodynamics of ideal and non ideal binary solutions. Gibbs Duhem equation, Duhem Margules equation. Different scales of activity coefficients for solutes and solvents.

Module 3: Unit 3: Kinetics **(10L)**

Brief review of collision theory & activated complex theory; ionic reaction, kinetic salt effect; steady state kinetics, kinetic & thermodynamic control of reactions; unimolecular reactions; chain reactions, fast reactions. Computational approach to understand the chemical kinetics of different ordered reactions.

Module 4: Unit 4: Electrochemistry **(10L)**

Activity and Activity coefficient of electrolytes, ionic strength, Debye Huckel theory of strong electrolytes. Debye Huckel limiting law, Mean ionic activity coefficient. Application of Debye Hückel theory to conductance bahaviour, Relaxation and electrophoretic effect, Debye-Hückel-Onsager equation and its derivation. Debye Falkenhagen effect. Wein effect.

Text books:

1. Physical Chemistry by G. W. Castellan.
2. P.W. Atkins, *Physical Chemistry*, 8th Edn., Wiley, New York, 2006

Reference texts:

1. J. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2B, 2nd Edn., Wiley, New York, 1998
2. Text-book of physical chemistry, by Samuel Glasstone
3. Physical Chemistry by Donald McQuaire
4. An Introduction to Electrochemistry – Samuel Glasstone
5. Chemical Kinetics – Keith J Laidler

Sl. No.	Content of the course	Module No.	%age of questions	Course outcome(CO)	CO	PO
1	Symmetry & group theory	Module 1/Unit-1	25	1.Effectively learn the group theory and its use for molecular term symbol.	CO1	PO1
2	Thermodynamics	Module 2/Unit-2	25	2.Information regarding thermodynamic properties of different systems which may be applied to understand the equilibrium conditions of chemical reactions	CO2	PO1
3	Kinetics	Module 3/Unit-3	25	3.Will be expertise to predict the reaction rate using computer softwere.	CO3	PO1
4	Electrochemistry	Module 4/Unit-4	25	4.Will be able to treat ionic reaction probably.	CO4	PO1

Analytical Techniques

Paper code: MSAC104
(3 Credit) (100 Marks)

Course Objectives:

1. To impart knowledge about spectroscopic techniques and solve structural problems based on UV-Vis, IR, ^{1}H-NMR, ^{13}C-NMR and mass spectral data.
2. Electron microscopy and mass spectroscopy will be learnt.
3. To impart knowledge about thermal analysis technique and associated methods
4. To learn separation techniques and data analysis using contemporary techniques

Module 1: Unit 1: Spectroscopy **(12L)**
Principles and applications of UV-Vis, Vibrational and Raman spectroscopy, Fluorescence and NMR spectroscopy in understanding chemical and biological interactions. Dynamic light scattering, Cyclic voltammetry, Circular dichroism.

Module 2: Unit 2: Electron Microscopy and Mass spectroscopy **(8L)**
SEM, TEM, AFM. Instrumentation, Mass spectral fragmentation of organic compounds, McLafferty rearrangement, structure determination.

Module 3: Unit 3: Thermal Methods **(6L)**
Theory and application of TGA, DSC and DTA.

Module 4: Unit 4: Separation Techniques and Data Analysis **(10L)**
HPLC, GC, gel electrophoresis for biological samples. Uncertainties, errors, mean, standard deviation, least square fit, testing the fit (C2 test, residual etc.). Signal to noise ratio.

Text books:

1. *Spectroscopy of Organic Compounds* by P.S. Kalsi, New Age International
2. Kemp, W. *Organic Spectroscopy* 3rd Ed., W. H. Freeman & Co. (1991).

Reference texts:

1. Silverstein, R. M., Bassler, G. C. & Morrill, T. C. *Spectroscopic Identification of Organic* Compounds John Wiley & Sons (1981).
2. Pavia, D. L.; Lampmann, G. M.; Kriz, G. S.; Vyvyan, J. R. *Introduction to Spectroscopy* Cengage Learning (2014).
3. *Organic Structures from spectra*; L. D. Field, S. Sternhell and J R Kalman, John Wiley & Sons Ltd., 2007

Sl. No	Content of the course	Module No.	%age of questions	Course Outcomes (CO)	CO	PO
1.	Spectroscopy	Module 1/Unit 1	30	1. Knowledge about spectroscopic techniques and solve structural problems based on UV-Vis, IR, ^{1}H-NMR, ^{13}C-NMR and mass spectral data.	CO1	PO2
2.	Electron microscopy and mass spectroscopy	Module 2/Unit 2	20	2. Electron microscopy and mass spectroscopy will be learnt.	CO2	PO2
3.	Thermal methods	Module	20	3. To impart knowledge	CO3	PO2

		3/Unit 3		about thermal analysis technique and associated methods.		
4.	Separation techniques and data analysis	Module 4/Unit 4	30	4. To learn separation techniques and data analysis using contemporary techniques.	CO4	PO2

Numerical Methods in Computational Chemistry

Paper code: MSAC105
(3 Credit)(100 Marks)

Course Objectives:

1. To learn about the linear and non-linear equations.
2. To know how linear and non-linear equations may be solved.
3. To learn to handel the matrix and determinant for scientific problem solution using computer.
4. To learn numerical methods to solve the differential equation and integration.
5. To learn the method of error calculation.
6. To learn different methods of numerical problem solution.

Module 1: Unit 1: Linear and non-linear equations **(10L)**

Linear and Non –Linear equations:Solution of Algebra and transcendental equations, Bisection, Falsi position and Newton-Rhapson methods-Basicprinciples-Formulae-algorithms.
Simultaneous equations:Solutions of simultaneous linear equations-Guass elimination and Gauss Seidel iterative methods-Basic principles-Formulae-Algorithms, Pivotal Condensation.

Module 2: Unit 2: Matrix and Determinants **(10L)**

Matrix and Determinants:Matrix Inversion, Eigen-values, Eigen-vector, Diagonalization of Real Symmetric Matrix by Jacobi's Method. First Principle approach.

Module 3: Unit 3: Programme to solve differential equation and integration **(10L)**

Interpolations: Concept of linear interpolation-Finite differences-Newton's and Lagrange's interpolation formulae-principles and Algorithms Numerical differentiation and integration: Numerical differentiation-algorithm for evaluation of first order derivatives using formulae based on Taylor'sseries, Numerical integration-Trapezoidal Rule, Simpson's 1/3 Rule, Weddle's Rule, Gauss Quadrature Formulae-Algorithms. Error in numerical Integration. Curve Fit: least square, straight line and polynomial fits.

Module 4: Unit 4: Numerical Solution of differential equations **(10L)**

Numerical Solution of differential Equations: Picards Method, Taylor's Series Method, Euler's Method, Modified Euler's Method, Runge-Kutta Method, Predictor-Corrector Method.

Text books:

1. V. Rajaraman, *Computer Oriented Numerical Methods*, PHI, 1993.
2. E. Balaguruswamy, *Numerical Methods*, Tata McGraw Hill, 2017.

Reference texts:

1. F. Acton, *Numerical Methods that Work*, Harper and Row, 1997.
2. S. D. Conte and C.D.Boor, *Elementary Numerical Analysis*, McGraw Hill, 2005.
3. S. S. Shastri, *Introductory Methods of Numerical Analysis*, PHI, 2012.

Sl. No	Content of the course	Module No	%age of questions	Course Outcomes (CO)	CO	PO
1	Linear and non-linear equations	Module 1/Unit-1	20	1.Will be able to handle linear and non-linear equations.	CO1	PO1
2.	Linear and non-linear equations	Module 1/Unit-1	20	2.Will be able to solve linear and non-linear equations.	CO2	PO1

3.	Matrix and Determinants	Module 2/Unit-2	10	3.Will be able to handle matrix and determinant using computer.	CO3	PO1
4.	Programme to solve differential equation and integration	Module 3/Unit-3	10	4.Will be able to write computer programme to solve differential equation and integration.	CO4	PO2
5.	Programme to solve differential equation and integration	Module 3/Unit-3	20	5.Will be able to calculate error of experimental results.	CO5	PO2
6.	Numerical Solution of differential Equations	Module 4/Unit-4	20	6.Will be able to use proper method for any kind of problem solution using numerical methods.	CO6	PO2

Lab Techniques for quantitative and qualitative analysis **Paper code: MSAC191**

(3 Credit) (100 Marks)

(40 Hr)

Course Objectives:

1. Characterization and analysis of organic compounds for identifying compounds.
2. To be able to synthesize organic compounds and separation of components in mixtures can be studied, which is of great use in different chemical fields.
3. To learn the techniques of purification of organic compounds from mixture.

Module 1: Unit 1: Identification of single organic compounds (solid/liquid) with one or more functional group(s) through preparation of derivatives.
Module 2: Unit 2: Organic preparations, including methods of purification (e.g., crystallization, steam distillation, vacuum distillation, sublimation, etc.).
Module 2: Unit 3: Chromatographic separation techniques to isolate single organic compound from mixture of compounds.

Reference texts:

1) *Vogel's textbook of practical organic chemistry* – Arthur Israel Vogel, B. S. Furniss
2) *Practical Organic Chemistry* - Frederick George Mann and Bernard Charles Saunders
3) *Advanced Practical Organic Chemistry* - N K Vishnoi
4) *Laboratory Manual of Organic Chemistry* - R. K. Bansal

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcomes (CO)	CO	PO
1.	Identification of functional groups in organic compounds	Module 1/Unit 1	30	1.Characterization and analysis of organic compounds for identifying functional groups can be learnt.	CO1	PO2
2.	Preparation of organic compounds	Module 2/Unit 2	30	2.Synthesis of organic compounds and separation of components in mixtures can be studied, which is of great use in different chemical fields.	CO2	PO2
3.	Purification of organic compounds	Module 2/Unit 3	40	3.Purification of organic compounds from mixture.	CO3	PO2

Computer Programming-I

Paper code: MSAC192
(3 Credit) (100 Marks)

Course Objectives: **(40 hr)**

1. To know how to use different operating systems of the computer.
2. To know the basic structure and principles of computer programming.
3. To learn object oriented computer programming.

Module 1: Unit-1: Basics of Programming
a. How to use different operating system - MS DOS, MS WINDOW, UNIX, Linux
b. Algorithm & flow chart of any programming
c. FORTRAN programming

Module 2: Unit-2: Advanced language programming
a. C/C^{++} Programming - Basics
b. Python programming – Basics
(For Python and C/C^{++} Programming data structure, Data Nature, Operator, statement, functions, object oriented programming, modules may be practised for small standard problems)

Reference texts:
1. *Linux Command Line and Shell Scripting Bible*, 3rd Edition, Wiley
2. *Compueter programming in FORTRAN 77*, Y. Rajaramann
3. *Essentials of Computational Chemistry: Theories and Models*, 2nd Edition, Christopher J. Cramer

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcomes (CO)	CO	PO
1.	Basics of Programming	Module 1/Unit 1	20	1. Will be able to handle different operating systems of computer.	CO1	PO1
2.	Basics of Programming	Module 1/Unit 1	30	2.Will be able to write simple FORTRAN programme.	CO2	PO1
3.	Advanced language programming	Module 2/Unit 2	20	3.Will be able to write C/C^{++} Programme	CO3	PO3
4.	Advanced language programming	Module 2/Unit 2	30	4.Will be able to write Python programme	CO4	PO3

Computer aided Stereo-chemical Analysis of Complex Chemical Reaction

Paper code:MSAC193

(2 Credit) (100 Marks)

(20 hr)

Course Objectives:

1. To know how to draw chemical structures using computer.
2. To know how to compute basic chemical properties of a compound.

Module 1: **Unit-1**: Analysis of Stereochemistry of single organic molecule and stereochemicaloutcome of complex chemical reaction using computer as analytical tool.
Module 2: **Unit-2**: Use of ChemOffice (Chemdraw 14.0/16.0 suite and Chemdraw 3D ultra) in order to determine most stable conformation of certain chemical structure.

Reference texts:

1. *User manual of ChemDraw*.

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcomes (CO)	CO	PO
1.	Analysis of Stereochemistry	Module 1/Unit 1	20	1.Will be able to draw the structure of organic compounds.	CO1	PO2
2.	Use of ChemOffice	Module 2/Unit 2	20	2.Will be able to predict R, S nomencleature of an organic compound.	CO2	PO2

Project-I

Paper code: MSAC194
(2 Credit)(100 Marks)

Students will be assigned with research articles for review, explanations with applications which will be submitted as a term paper to the department programme coordinator before the start of semester I examination. A presentation will be made and delivered in presence of the departmental faculty members for assessment.

AUDIT COURSE:

Paper code: MSAC181

An audit course in chemistry will be chosen from MOOC's basket between Semester 1 and Semester 3 and the certificate of successful course completion has to be submitted before the exam of 3rd Semester to the competent authority. The audit course will be designed in keeping with the requirements of the course and will be of minimum four (04) weeks duration.

SEMESTER - II

Quantum Chemistry

Paper code: MSAC201
(3 Credit) (100 Marks)

Course Objectives:

1. To know the details of quantum numbers.
2. To know how to calculate different quantum numbers.
3. To know how to solve the wavefunction of a system by purterbation method.
4. To know different quantum numbers.
5. To know molecular structure theory.

Module 1: Unit 1: Recapitulations of the background (12L)
Origin of the quantum theory. Blackbody radiation and Heisenberg uncertainty principle, Postulates of quantum mechanics and Schrödinger equation; Operator algebra & its application on some model systems viz., free-particle and particle in a box, three dimensional system, tunnelling effect, Hermitian operator, Laplacian operator, the harmonic oscillator, hermite polynominals; the rigid rotator, and the hydrogen atom, hydrogen like atom, Zeemann effect.

Module 2: Unit 2: Perturbation Theory (8L)
Perturbation theory for non-degenerate and degenerate states and its applications. The variation theorem and its applications to the helium atom.

Module 3: Unit 3: Generalized Angular Momenta and Spin (8L)
Generalized angular momentum, basis functions and representation of angular momentum operators; Electron Spin, Electron's magnetic Moment and Spin Angular Momentum. Ladder operators, Gyromagnetic Ratio and Bohr Magneton and the g - factor.

Module 4: Unit 4: Atomic and Molecular Structure (12L)
Many electron wave functions, Pauli exclusion principle, Helium atom, atomic term symbols. The self-consistent field method. Slater-type orbitals. Valence-bond (VB) and Molecular orbital (MO) treatment for homonuclear and heteronuclear diatomic molecules. Hückel molecular orbital theory; application of quantum mechanics to molecular spectroscopy, introduction to density functional theory.

Text books:

1. *Quantum Chemistry*, I.N. Levine, 5th edition, Pearson Educ., Inc. New Delhi (2000).
2. *Chemical Applications of Group Theory*, F. A. Cotton, John Wiley & Sons (2008).

Reference texts:

1. *Physical Chemistry: A Molecular Approach*, D. A. McQuarrie, and J. D. Simon, Viva Books (2011).
2. *Valence Theory*, J.N. Murrell, S.F.A. Kettle and J. M. Tedder, 2nd edition, John Wiley (1965).
3. *Introductory Quantum Chemistry*, A.K. Chandra, 4th Edition, Tata Mcgraw Hill (1994).
4. *Molecular Symmetry and Group Theory*, R. L. Carter, J. Wiley (1998).
5. *Group Theory and Chemistry*, D. M. Bishop, Dover Publications (1993).
6. *Quantum Chemistry*, J. P. Lowe, and Peterson, K., Academic Press (2005).

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcomes (CO)	CO	PO
1.	Recapitulations of the background	Module/Unit-1	10	1.Will be familiar with different quantum numbers.	CO1	PO1
2.	Recapitulations of the background	Module 1/Unit-1	15	2.Will be able to calculate the quntum number of an electron in a particular state.	CO2	PO1
3.	Perturbation Theory	Module 2/Unit-2	25	3.Will be able to findout the wave function of any chemical system.	CO3	PO1
4.	Generalized Angular Momenta and Spin	Module 3/Unit-3	25	4.Will be able to relate the spectra of a system with its electronic structure.	CO4	PO1
5.	Atomic and Molecular Structure	Module 4/Unit-4	25	5.Will be able to learn about the electronic structure of a molecule.	CO5	PO1

Statistical Mechanics

Paper code: MSAC202
(3 Credit)(100 Marks)

Course Objectives:

1. To gain concept of different ensembles and partition functions help in calculating specific heat of solids.
2. To impart knowledge on distribution and fluctuations of parameters in different systems can be learnt, which will help in understanding fluctuations in macroscopic observables.
3. To impart knowledge on different thermodynamic properties in various systems can be known which have applications in real systems.
4. Properties of elctrons in metals can be known and applications in real systems can be done.

Module 1: Unit 1: Probability Theory And Distribution (8L)
Mathematical and thermodynamic probability. Distributions and Averages, Cumulants and Fluctuations, The Central Limit Theorem Distributions & Fluctuations. Most probable distribution, independent sub-systems and distinguishability.

Module 2: Unit 2: Basic Thermodynamics (10L)
Basic Thermodynamics: Review of concepts, The Laws of Thermodynamics, Partition Function: Equipartition of energy principles, redsidual entropy. Classical rotational, vibrational and translational partition functions. Application of partition functions to specific heat of solids and chemical equilibrium. Real gases.

Module 3: Unit 3: Review of Classical Mechanics And Partition Functions (10L)
Concept of Ensembles and Phase Space, Classical and Quantum Equivalence of Ensembles, Fluctuations of Macroscopic observable. Liouville's Theorem-Ergodic hypothesis, Equilibrium Statistical Mechanics and it's ensembles. Legendre transforms, The Maxwell relations, the Gibbs-Duhem equation and extensive functions, intensive functions.

Module 4: Unit 4: Quantum Statistics (8L)
Bose-Einstein distribution: Einstein condensation. Thermodynamic properties of ideal BE gas. Fermi-Dirac distribution: Degenerate Fermi gas. Electron in metals.

Text books

1. Kerson Haung, *Statistical Mechanics*, Wiley, 2nd Ed. (2008).
2. R. K. Pathria and P. D. Beale, *Statistical mechanics*, Elsevier, 3rd Ed (2011).

Reference texts:

1. D. A. Mcquarrie, *Statistical Mechanics*, University Science Books (2011).
2. D. Chandler, *Introduction to Statistical Mechanics*, Oxford University Press (1987).

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcomes (CO)	CO	PO
1.	Probability theory and distribution	Module 1/Unit 1	20%	1. Knowledge on distribution and fluctuations of parameters in different systems can be learnt, which will help in understanding fluctuations in macroscopic observables	CO1	PO1
2.	Basic	Module	30%	2. Knowledge on different	CO2	PO1

	Thermodynamics	2/Unit 2		thermodynamic properties in various systems can be known which have applications in real systems		
3.	Review of Classical Mechanics and Partition Functions	Module 3/Unit 3	30%	3. Fluctuations of observables in different systems can be estimated which has wide applications.	CO3	PO1
4.	Quantum Statistics	Module 4/Unit 4	20%	4. Properties of elctrons in metals can be known and applications in real systems can be done.	CO4	PO1

Organic Chemistry-II

Paper code: MSAC203
(3 Credit)(100 Marks)

Course Objectives:

1. To gain knowledge on various metal-catalyzed coupling reactions, reducing agents, oxidizing agents, and their applications in organic synthesis
2. To acquire knowledge on organic spectroscopic techniques and solve problems and structural anylaysis
3. To impart knowledge on synthesis and utility of various heterocyclic compounds
4. To acquire knowledge of basic principles of photochemistry and advanced photochemical reactions

Module 1: Unit 1: Reagents in Organic Synthesis **(10L)**

Diborane, lithium aluminium hydride, sodium borohydride, selenium-di-oxide, osmium tetroxide, phenyl isothiocyanate, *N*-bromosuccinimide, lead tetraacetate, dicyclohexylcarbodiimide (DCC), pyridinium cholorochromate (PCC), Swern oxidation, p-toluenesulphonyl chloride, trifluoroacetic acid, lithiumdiisopropylamide (LDA), 1,3-dithiane (reactive umpolung), crown ethers, trimethylsilyl iodide, Gilman reagent, dichlorodicyanobenzoquinone (DDQ), lithium dimethylcuprate, tri-n-butyltin hydride, di-tert-butoxydicarbonate, dihydropyran, phase transfer catalysts, Wilkinson's catalysts, Peterson synthesis and diethylaluminium cyanide, IBX.

Module 2: Unit 2: Organic Spectroscopy **(10L)**

Advanced Techniques and Applications of NMR: ^{1}H and ^{13}C NMR principles, rules for ^{13}C calculations, principles of decoupling, gated and inverse gated decoupling techniques, NOE, relaxation processes, population transfer, selective polarization transfer, NMR shift reagents and their applications, basic two-dimensional sequence.

Module 3: Unit 3: Heterocycles **(10L)**

Synthesis and reactivity of furan, thiophene, pyrrole, azoles, pyridine, indole, quinoline, isoquinoline, pyrimidine, purine, coumarin and flavones-structure, synthesis, properties and reactions. Skraup synthesis, Fischer indole synthesis and Pachmann coumarin synthesis, alkaloids-sources and classification, structural elucidation by chemical degradation, total synthesis of quinine, morphine, reserpine, papaverine and nicotine (Any two).

Module 4: Unit 4: Photochemistry **(10L)**

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, cis-trans isomeriation, Paterno-Buchi reaction, Norrish type I and II reactions, photoreduction of ketones, di-pi-methane, oxo di-pi methane and aza di-pi methane rearrangements, Barton reaction, Hofmann-Loefflar-Freytag reactions, photochemistry of arenes, SRN^{1} reaction, photooxidation, Photoreaction in solid state. Method of generation and detection of radicals (ESR), radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, synthetic applications: cyclisation of radicals including various ring expansion, ring contraction, remote functionalisation and radical fragmentation reaction. Photochemical reaction using UV, Sunlight and LED light etc. Photochemical smog.

Text books:

1. J. March, *Advanced Organic Chemistry*, 5th edition, Wiley-Intersciences, New York (2003).
2. F.A.Carey and R.J. Sundberg, *Advanced Organic Chemistry, Part A and Part B*, 5th edition, Plenum Press, New York (2005).

Reference texts:

1. T.H. Lowry and K.S. Richardson, *Mechanism and Theory in Organic Chemistry*, 2nd edition, Harper and Row Publishers (1981).
2. R.K. Mackie and D.M. Smith, *Guide book to Organic Synthesis*, 2nd edition, ELBS Publications, London (1998).
3. Horspool, W. M. *Aspects of Organic Photochemistry* Academic Press (1976).
4. *Heterocyclic Chemistry*: Joule, John A., Mills, Keith.
5. *Absorption spectroscopy of organic molecules*- V.M. Parikh
6. R.P.Wayne, "*Principles and Applications of Photochemistry*", Oxford University Press
7. C.H.Dupuoy, and O.L.Chapman, "*Molecular Reactions and Photochemistry*", Prentice Hall
8. *Essentials of molecular photochemistry*, A. Gilbert and J. Baggott. Blackwell Scientific Publication.
9. *Introductory photochemistry*. Cox and T. Camp Mc Graw –Hill
10. *Organic photochemistry* J. Coxon and B. Hallon Cambridge University press.

Sl. No	Content of the course	Module No.	%age of questions	Course Outcomes (CO)	CO	PO
1.	Reagents in organic synthesis	Module-1/ Unit-1	25%	1. Knowledge on various metal-catalyzed coupling reactions, reducing agents, oxidizing agents, and their applications in organic synthesis.	CO1	PO1
2.	Organic spectroscopy	Module-2/Unit-2	25%	2. Acquire knowledge on organic spectroscopic techniques and solve problems and structural anylaysis.	CO2	PO1
3.	Heterocycles	Module-3/Unit-3	25%	3. Learn about synthesis and utility of various heterocyclic compounds.	CO3	PO1
4.	Photochemistry	Module-4/Unit-4	25%	4. Knowledge of basic principles of photochemistry and advanced photochemical reactions.	CO4	PO1

Nano Science and Technology

Paper code: MSAC204
(3 Credit)(100 Marks)

Course Objectives:

1. To learn about synthesis of nano materials of various elements having different properties, which has diverse industrial applications.
2. To learn structure and characterization of nano materials and study for their applications in drug delivery processes.
3. To know symmetry in molecules and different properties of nano materials which help in applications in medical fields.

Module 1: Unit 1: Introduction to Nanoscience and Nanotechnology (10L)
Basic problems and limitations - opportunities of nano scale-evolution of band structures andFermi surface. Nanoparticles through homogeneous and heterogeneous nucleation-Growth controlled by surface and diffusion process- Oswald ripening process - influence of reducing agents-solid state phase segregation- grain growth and sintering precipitation in solid solutionhumerothery rule. Carbon Nanotubes (CNT) - Metals (Au, Ag, Pd, Cu) - Metal oxides (TiO2, CeO2, ZnO, MgO) -Semiconductors (Si, Ge, CdS, ZnSe). Classifications of nanomaterials-zero dimensional - one dimensional - two dimensional - three dimensional nanostructures - Quantum dots - Quantum wire, Quantum well-semiconductors and ceramics.

Module 2: Unit 2: Special nanomaterials (10L)
Carbon fullerenes-fullerene derived crystals-carbon nanotubes. Micro and Mesoporous material ordered mesoporous materials, Random mesoporous materials-crystalline microporous materials.Core/Shell structures, Metal oxide structures, Metal polymer structures, Intercalation compounds-nanograined materials. Nanomaterials in drug delivery.

Module 3: Unit 3: Materials Structure and Properties (10L)
Space lattice and unit cells, crystal system, Symmetry operation, Structures of common metallic, Semiconductor ceramic and superconductor materials, Miller Indices, Packing fractions, Formation of dangling bonds-atom like behavior of nanomaterials-physicochemical properties. Optical properties of nanomaterials-semiconductor-metal nanoparticles-Electrical and electronic properties, Thermal properties-Ferro electric properties-mechanical and magnetic properties.

Module 4: Unit 4: Organic nanomaterials, nanoelectronics and engineering (8L)
Organic nanoelectronics. Advanced nanomaterials for applications. Nanosystems engineering to design, develop, and characterize materials on the nanoscale. Nanoparticles for Environment, Engineering, and Nanomedicine.

Text books:

1. *Introduction to Nanoscience and Nanotechnology*, By Gabor L. Hornyak, H.F. Tibbals, Joydeep Dutta, John J. Moore
2. *Nanostructures and Nanomaterials: Synthesis, Properties, and Applications*, By Guozhong Cao, Ying Wang.

Reference texts:

1. *Organic Nanomaterials: Synthesis, Characterization, and Device Applications*, By Tomas Torres, Giovanni Bottari
2. *Nanochemistry: A Chemical Approach to Nanomaterials*, By Geoffrey A. Ozin, André C. Arsenault, Ludovico Cademartiri
3. T. Pradeep, *Nano The Essentials: Understanding Nanoscience and Nanotechnology*.

Sl. No	Content of the course	Module No	%age of questions	Course Outcomes (CO)	CO	PO
1	Introduction to nanoscience and nanotechnology	Module 1/Unit 1	30%	1. Synthesis of nano materials of various elements having different properties can be learnt, which has diverse industrial applications	CO1	PO1
2.	Special nanomaterials, nanoelectronics and engineering	Module 2/Units 2 and 4	40%	2. Structure and characterization of Nano materials will be studied for application in drug delivery processes	CO2	PO2
3.	Material structures and properties	Module 3/Unit 3	30%	3. Symmetry in molecules and different properties of nano materials will be known which help in applications in medical fields	CO3	PO3

Applications of Artificial Intelligence and Machine Learning in Chemistry

Paper code: MSAC205

(2 Credit)(100 Marks)

Course Objectives:

1. To learn the basics of ML approach and its concepts from problem setting to evaluating the goodness of a model.
2. To learn how ML is used in contemporary chemistry and can analyze and evaluate a chemistry-related ML article.

Module 1: Unit 1: Introduction to AI/ML **(10L)**

Introduction to AI/ML, Math review, Regression and Classification, Support Vector Machine, Multi-Layer Perceptron, Convolutional Neural Network (CNN), Molecular graph and Graph Neural Network (GNN), SMILES and Recurrent Neural Network (RNN), Graph Neural Network and Message Passing Neural Network (MPNN), Variational Autoencoder (VAE), Reinforcement Learning (RL).

Module 2: Unit 2: Applications in Chemistry **(10L)**

Application of machine learning in drug discovery, chemical synthesis and analysis of spectra, nanomaterials and biology interface, designing of functional materials, inorganic materials, challenges and opportunities of AI/ML in chemistry.

Text books:

1. *"Applications of Artificial Intelligence in Chemistry*" By Hugh M. Cartwright. Oxford University Press: Oxford, England, 1993.
2. "Machine Learning in Chemistry: The Impact of Artificial Intelligence" By Hugh M. Cartwright.

Reference texts:

1. "Artificial Intelligence: The Future for Organic Chemistry?"
Franck Peiretti, Jean Michel Brunel, *ACS Omega* 2018, 3, 10, 13263–13266.
2. "Artificial intelligence in chemistry." N.A.B Gray Analytica Chimica Acta, 1988, 210, 9-32.
3. "Synthetic organic chemis try driven by artificial intelligence."
A. Filipa de Almeida, Rui Moreira,Tiago Rodrigues, *Nature Reviews Chemistry*, 2019 3, 589–604.
4. "Machine learning for chemical discovery" Alexandre Tkatchenko
Nature Communications 2020, 11, 4125.

Sl. No	Content of the course	Module No	%age of questions	Course Outcomes (CO)	CO	PO
1	Introduction to AI/ML	Module 1/Unit 1	50%	1. To learn the basics of ML approach and its concepts from problem setting to evaluating the goodness of a model.	CO1	PO2
2.	Applications in Chemistry	Module 2/Unit 2	50%	2. To learn how ML is used in contemporary chemistry and can analyze and evaluate a chemistry-related ML article.	CO2	PO3

Natural Products and Medicinal Chemistry

Paper code: MSAC206
(3 Credit)(100 Marks)

Course Objectives:

1. To be able to define structure and synthesis of amino acids, peptides and nucleic acids.
2. To learn basic concepts and application of natural products and synthetic molecules in medicinal chemistry.
3. To learn lead drugs and to describe the biogenesis and biosynthetic studies of different classes of drugs.

Module 1: Unit 1: Natural products **(10L)**

Introduction, isoprene rule, general methods of isolation, structure elucidation and synthesis of some representative members of mono and sesquiterpenes. Biogenesis and biosynthesis of mono, sesqui- and di-terpenoids. Definition and classification, general methods of isolation and structure elucidation, structure and synthesis of ephedrine, piperine, nicotine and papaverine.

Introduction, classification, sources of occurrence and role of steroids (including steroidal hormones) in human body. Chemistry of oestrone.

Structure, stereochemistry, biogenetic precursors and medicinal importance of alkaloids from terrestrial and marine sources with special reference to morphine, quinine, reserpine, yohimbine and lysergic acid.

Module 2: Unit 2: Proteins and Nucleic Acids **(6L)**

Classification, structure and synthesis of amino acids, peptides. Merrifield solidphase peptide synthesis, structure determination, peptide sequence and synthesis of - primary, secondary, tertiary and quaternary structures. Nucleic acids, structure and synthesis of DNA. Structure and synthesis of RNA, WC Model.

Module 3: Unit 3: Introduction to Medicinal Chemistry **(10L)**

Chemical basis of disease states, definition and classification of drugs. Concept of pharmacokinetics and pharmacodynamics. Methods of drug administration, drug metabolism and drug excretion, enzyme inhibitors, receptors, chemical messengers, agonists and antagonists. Drug dosing and drug half-life, drug tolerance and physical dependence, drug potency, drug efficacy, dose response curves and therapeutic index (LD-50 & CD-50). Development of new drugs, concepts of prodrugs and soft drugs, pharmacophores, lead compounds.

Definition of vitamins and coenzymes, classification of vitamins, mechanism of function with synthesis of vitamin A, B1, B6 and folic acid, etc.

Module 3: Unit 4: Advanced Medicinal Chemistry **(10L)**

Mechanism of action and synthesis of some non-steroidal anti-inflammatory drugs (NSAIDs). Molecular modelling and energy minimization; molecular properties, conformational analysis, Docking procedures, *De novo* design, Molecular recognition, Receptor based molecular modeling, QSAR studies, antineoplastic agents, cardiovascular drugs, local anti-infective drugs, Antimalarial, Anticholenergic and CNS-active drugs and psychotic drugs (diazepam, oxazepam, chlorpromazine, librium, alprazolam, barbiturates etc.).

Text books:

1. Gringauz, A. *Introduction to Medicinal Chemistry: How Drugs Act and Why?* John Wiley & Sons (1997).
2. Patrick, G. L. *Introduction to Medicinal Chemistry,* Oxford University Press (2001).

Reference texts:

1. Lemke, T. L. & William , D. A., Foye's *Principles of Medicinal Chemistry*, 5th Ed., USA, (2002).

2. D. Sriram , P. Yogeswari, *Medicinal Chemistry*, Pearson Education India, 2010.
3. C.O. Wilson, J.M. Beale, J.H. Block, *Textbook of Organic Medicinal and Pharmaceutical Chemistry*, 12th Edn., Lippincott Williams and Wilkins, 2010
4. S. S. Kadam, *Principles of Medicinal Chemistry*, Vol. I & II, Pragati Books, 2008

Sl. No	Content of the course	Module No	%age of questions	Course Outcomes (CO)	CO	PO
1	Natural Products	Module 1/Unit 1	30	1. To learn basics of lead drugs and to describe the biosynthetic studies of different classes of drugs.	CO1	PO1
2.	Proteins and nucleic acids	Module 2/Unit 2	20	2. To acquire knowledge on structure and synthesis of amino acids, peptides and nucleic acids.	CO2	PO1
3.	Introduction and advanced medicinal chemistry	Module 3/Units 3 and 4	50	3. To acquire knowledge on concepts of synthetic molecules in medicinal chemistry.	CO3	PO3

Computational Methods in Chemistry

Paper code: MSAC291
(3 Credit)(100 Marks)

Course Objectives:

1. To familiar with the geometry optimization.
2. To know how to use computational tool to compute the properties of a compound.
3. To know how we could handel the data to analyse using computer.

Module 1: Unit-1: Computational Lab **(20hr)**
Simulation and structures and geometry optimisation with the commercial programs like "Materials Studio" (Forcite, Force Field: COMPASS), Gaussian.
Module 2: Unit-2: Computational Lab **(10hr)**
Computational studies on opto-electronic and charge transport properties in conjugated systems. Other computational application introducing "ChemCraft", "Gaussian", "SCM ADF" softwares GAMMES.
Module 3: Unit-3: Computational Lab **(10hr)**
Plotting, analysis and interpretation of data from UV-Vis or Fluorescence spectrophotometry using Origin.

Reference texts:

1. *User guide of Gaussian*.
2. *Molecular Dynamics Simulation: Fundamentals and Applications*, Kun Zhou and Bo Liu, Academic Press Inc (1 November 2020)

Sl. No	Content of the course	Module No	%age of questions	Course Outcomes (CO)	CO	PO
1	Computational Lab	Module 1/Unit 1	20	1.Will be able to draw structure and optimize it using DFT.	CO1	PO2
2.	Computational Lab	Module 2/Unit 2	40	2.Will be able to compute physical and chemical properties of a compound.	CO2	PO3
3.	Computational Lab	Module 3/Unit 3	40	3.Will be able to plot and analyse data with the help of computer.	CO3	PO3

Advanced Chemistry Laboratory

Paper code: MSAC292
(3 Credit)(100 Marks)

Course Objectives:

1. To acquire knowledge of laboratory techniques for organic synthesis and characterization.
2. To learn synthetic procedures: aqueous workup, distillation, reflux, separation, isolation, and crystallization.
3. To gain knowledge about starting materials, functional groups, mechanism, and typical reaction conditions.

Module 1: **Unit-1: Some important techniques in practical organic chemistry**: **(8hr)**
Recrystallization, mixed melting point, drying of solvents and steam distillation.

Unit-2: Preparation of **(16hr)**
i) Methyl orange ii) Coumarin iii) Pyrazolone iv) Azalactone

Unit-3: Preparation of **(16hr)**
i) Benzanilide by Beckmann's rearrangement:
(a) Preparation of benzophenone oxime
(b) Beckmann's rearrangement to benzanilide
ii) Benzilic acid from benzoin:
(a) Benzil from benzoin
(b) Benzilic acid from benzyl
iii) Anthranilic acid from phthalic anhydride:
(a) Phthalimide from Phthalic anhydride
(b) Hoffmann's rearrangement to anthranilic acid
iv) m-Nitroaniline from Nitrobenzene:
(a) m-Dinitrobenzene from Nitrobenzene
(b) m-Nitroaniline from m-Dinitrobenzene

Reference texts:
1) *Vogel's textbook of practical organic chemistry* – Arthur Israel Vogel, B. S. Furniss
2) *Practical Organic Chemistry* - Frederick George Mann and Bernard Charles Saunders
3) *Advanced Practical Organic Chemistry* - N K Vishnoi
4) *Laboratory Manual of Organic Chemistry* - R. K. Bansal

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcomes (CO)	CO	PO
1.	Some important techniques in practical organic chemistry	Module 1/Unit 1	20%	1. Will learn laboratory techniques for organic synthesis and characterization.	CO1	PO2
2.	Preparation of organic compounds	Module 1/Unit 2	40%	2. Learn synthetic procedures: aqueous workup, distillation, reflux, separation, isolation, and crystallization.	CO2	PO3

3.	Preparation of organic compounds via multistep synthesis	Module 1/Unit 3	40%	3. Gain knowledge about starting materials, functional groups, mechanism, and typical reaction conditions.	CO3	PO3

Project-II

Paper code: MSAC293
(3 Credit)(100 Marks)

Students will select a research topic, inline with the topics covered in their MSc program and will submit a review report on that topic to the department programme coordinator before the start of semester II examination. A presentation will be made and delivered in presence of the departmental faculty members for assessment.

SEMESTER - III

Bioorganic, Supramolecular and Green Chemistry

Paper code: MSAC301
(3 Credit)(100 Marks)

Course Objectives:

1. Able to describe Supra molecules and their interactions.
2. Aquire knowledge on Bio-organic molecules and their applications.
3. Able to apply green chemistry for synthetic applications and catalytic reactions.

Module 1: Unit -1: Supramolecules: Interactions (10L)

Basic concepts of supramolecular chemistry, different noncovalent forces (e.g. H-bonding, cation-π, anion-π, π-stacking, hydrophobic, hydrophilic interactions etc.) leading to strong bonding of guest molecules to the hosts, thermodynamics of host-guest complexation, solvent effects and salt effects in complexation, design principle of host molecules.

Module 2: Unit -2: Supramolecules: Chracterization and Applications (10L)

Experimental techniques for characterization of host – guest complexation, examples of different design-based receptor molecules for cation, anion and neutral molecules binding, chiral recognition with examples, supramolecular devices (optical and electrochemical) and molecular switches, self-organization process-template association and supramolecular synthesis, self-replication and autocatalysis, supramolecular reactivity and catalysis, transport processes and carrier design, supramolecular gel.

Module 3: Unit -3: Bioorganic Chemistry (10L)

Structure and utility of natural and unnatural compounds, carbohydrates, biopolymers, nucleic acids, amino acids, peptides, drug molecules. Enzymes-classifications, function, enzyme model, kinetic of enzyme catalysis, serine and cysteine proteases, co-factors, co-enzymes and metalloproteins. Drug – Receptor binding and Bioorganic compounds for drug delivery and bio-signalling.

Module 4: Unit -4: Green Chemistry (8L)

Introduction, Principles & Concepts of Green Chemistry. Catalysis and Green Chemistry: Oxidations and Reductions, C-C Bond Formation. Environmentally Benign Solutions (Focus on water, ionic liquid, fluorous solvents and super critical CO_2).

Text books:

1. Steed, J. W.; Turner, D., R.; Wallace, K. J., *Core Concepts in Supramolecular Chemistry and Nanochemistry*, John Wiley & Sons, West Sussex (2007).
2. Steed, J. W.; Atwood, J. L., *Supramolecular Chemistry*, 2nd Ed., John Wiley & Sons, West Sussex (2009).

Reference texts:

1. Cotton, F. A.; Bochmann, M.; Murillo, C. A.; Wilkinson, G., *Advanced Inorganic Chemistry*, 6th Ed., Wiley India, New Delhi (2007).
2. Ariga, K.; Kunitake, T., *Supramolecular Chemistry: Fundamentals and Applications*, Springer, Heidelberg (2006).
3. Lehn, J.-M., *Supramolecular Chemistry: Concepts and Perspectives*, Wiley India, New Delhi (2014).

Sl. No	Content of the course	Module No.	%age of questions	Course Outcome (CO)	CO	PO
1.	Supramolecular chemistry	Module 1 & 2/Unit 1, Unit 2	50%	1.To gain knowledge in bonding in supra molecules and their formations will help in understanding supra molecular devices and molecular switches	CO1	PO1
2.	Bio-organic Chemistry	Module 3/Unit 3	30%	2.To learn structure and utility of natural and unnatural organic compounds which will help in understanding drug-receptor binding for applications in drug delivery processes.	CO2	PO1
3.	Green Chemistry	Module 4/Unit 4	20%	3.To be able to apply green chemistry in chemical reactions and environmentally benign solutions.	CO3	PO1

Biochemistry and Bioinorganic Chemistry

Paper code:MSAC302
(3 Credit) (100 Marks)

Course Objectives:

1. To gain knowledge on different interactions and energy change in cells can be understood. This will help in biochemical applications.
2. To gain knowledge on different methods of Preparation of organometallic compounds will be known and may be applied to industry.
3. T learn structure and bonding involved in supramolecules can be determined. These molecules are required in industry.
4. Transport of different elements and energy within cells can be determined which has applications in pharmaceutical field.

Module 1: Unit 1: Basics of Biochemistry **(8L)**

Principles of biophysical chemistry, Thermodynamics, Colligative properties, Stabilizing interactions: Van der Waals, Electrostatic, Hydrogen bonding, Hydrophobic interaction, etc.Composition, structure, function and metabolism of Carbohydrates, Lipids, Amino Acids and Nucleotides. Bioimaging.

Module 2: Unit 2: Organometallic Compounds **(10L)**

Metal carbonyls-synthesis, structure and bonding in mononuclear and polynuclear carbonyls with and without bridging, metal carbonyl hydrides and metal carbonyl clusters. Complexes with linear π donor ligands: olefins, acetylenes, dienes and allyl complexes. Catalysis by organometallic compounds-hydrogenation, hydroformylation and polymerisation reactions. (Wilkinson's catalyst, Ziegler-Natta catalyst & Synthetic gasoline should be included among various examples) and various others applications. Application of C-H, C-X activation and functionalization.

Module 3: Unit 3: Metal-Organic Framework and Covalent Organic Framework **(8L)**

Macrocycles and supramolecules non-covalent forces and interactions in supramolecules: crown ethers, cryptates, cryptands, carcerands, calixarenes, cyclodextrins, fullerenes, dendrimers, rotaxanes, self-assembly and preorganization, coordination driven self-assembly of supramolecular two and three dimensional architectures, host-guest chemistry, metal-organic frameworks, covalent-organic frameworks and their applications.

Module 4: Unit 4: Bioinorganic Chemistry **(10L)**

Principles of coordination chemistry related to bioinorganic chemistry, Essential and trace metal ions in biological systems, Porphyrin and related ligands, ATP as energy source, oxidative phosphorylation and phosphorylation of glucose. Transport and storage of dioxygen: Structure and function of hemoglobin, myoglobin, hemocyanin and hemerythrin. Synthetic oxygen carriers. Mechanism of gas transport (e.g.- NO_2, CO_2 etc).

Text Books:

1. F. A. Cotton, G. Wilkinson, C. A, Murillo, and M. Bochmann *Advanced Inorganic Chemistry*, 6th Edition Wiley-Interscience: New York, 1999.
2. D. F. Shriver, P. W. Atkins, C. H. Langford, *Inorganic Chemistry*, 3rd Ed. ELBS, 1999.

Reference texts:

1. J. W. Steed, J. L. Atwood, *Supramolecular Chemistry*, 2nd edition, John Wiley & Sons Ltd., (2009)
2. B. Douglas, D. McDaniel, J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Ed., Wiley.
3. Berg, J.M., Tymoczko, J.L. and Stryer, L. (2010). *Biochemistry*. W.H. Freeman & Company. USA.

4. Brown, T.A. (2006). *Gene Cloning and DNA analysis: In Introduction*. Blackwell Publishing Professional. USA.
5. Haynie, D.T. (2007). *Biological thermodynamics*.Cambridge University. UK.
6. Mathews, C.K., Van Holde, K.E. and Ahern, K.G. (2000). *Biochemistry*. Oxford University Press Inc. New York.
7. J.E. Huheey, Ellen A. Keiter and Richard L. Keiter "*Inorganic Chemistry, Principles of structure and Reactivity*", 4th Ed., Harper Collin College Publishers, 1993

Sl. No	Content of the course	Module No.	%age of questions	Course Outcomes (CO)	CO	PO
1.	Basics of biochemistry	Module-1/ Unit-1	20%	1. Different interactions and energy change in cells can be understood. This will help in biochemical applications.	CO1	PO1
2.	Organometallic compounds	Module-2/Unit-2	30%	2. Different methods of Preparation of organometallic compounds will be known and may be applied to industry.	CO2	PO1
3.	Metal-organic framework and covalent organic framework	Module-3/Unit-3	20%	3. Structure and bonding involved in supramolecules can be determined. These molecules are required in industry.	CO3	PO3
4.	Bioinorganic chemistry	Module-4/Unit-4	30%	4. Transport of different elements and energy within cells can be determined which has applications in pharmaceutical field.	CO4	PO3

Research Methodology

Paper code:MSAC303
(3 Credit) (100 Marks)

Course Objectives:

1. Literature survey and definition of a research problem.
2. Design of research plan and techniques to solve problem.
3. Different software for computer programming.
4. Analysis of data from experimental work.

Module 1: Unit 1: Introduction to Research **(6L)**

Definition of problem: Necessity of defining problem, Technique involved in defining a problem. Surveying the available literature. Techniques involved in solving the problem: Different methods used to solve a problem.

Module 2: Unit 2: Design of Research Plan **(12L)**

Research Design: Subject of study; Place of study; Reason of such study; Type of data required; Method of data collection; Periods of study; Style of data presentation.

Developing a research plan: Research objective; Information required for solving the problem; each major concept should be defined in operational terms; an overall description of the approach should be given and assumption if considered should be clearly mentioned in

Research plan; the details of techniques to be adopted.

Methods of data collection: Experimental methods.

Module 3: Unit 3: Applications of Softwares in Research **(10L)**

Computer: Basic of Computer Operating System: Using Windows – Directory structures – command structure (Document preparation, EXCEL, PowerPoint Presentation).

Word Processing: Basics of Editing and Word **Applications of Softwares in Research** processing.

Numerical analysis. Figure Plotting: Figure insertions in documents.

Web Browsing for Research: Usage of Webs as a tool for scientific literature survey.

Module 4: Unit 4: Data Analysis **(8L)**

Analysis of data: Various measures of relationship often used in research studies, Correlation coefficients. Chi-Square test: Definition of chi-square test. Significance in Statistical analysis.

Error Analysis: Basics of a measurement and its interpretation, central tendency and dispersion (variance), correlation coefficient; Usage of packages (e.g. ORIGIN; EXCEL) for data analysis.

Curve Fitting: Linear and Non-linear fitting of data. Rudimentary elements to design the experiments.

Text book:

1. Research Methodology : Methods and Techniques by C.R. Kothari.

Reference Texts:

1. Research Design by John W. Creswell.

Sl.No	Content of the course	Module No.	%age of questions	Course Outcomes (CO)	CO	PO
1.	Introduction to Research	Module-1/ Unit-1	20%	1. To be able to search the Literature and define a research problem.	CO1	PO1
2.	Design of Research Plan	Module-2/Unit-2	30%	2. Capable of designing a research plan and techniques to solve problem	CO2	PO2
3.	Applications of Softwares in Research	Module-3/Unit-3	30%	3. Apply different software for computer programming.	CO3	PO2
4.	Data Analysis	Module-4/Unit-4	20%	4.Able to analyze of data from experimental work	CO4	PO1

(Elective I) A. Photochemistry & Spectroscopy

Paper code: MSAC304A
(3 Credit) (100 Marks)

Course Objectives:

1. To learn changes in energy levels of a molecule after absorption of radiation to understand the effect of sunlight on living systems.
2. To gain knowledge about manufacture of laser for use in different field.
3. To know life time in the excited states of molecules which helps in predicting the reactions at excited state.
4. To learn characterization of the molecules and their applications for use in different field.

Module 1: Unit 1: Photophysical processes in molecules (8L)

Jablonski diagram, Fluorescence and Phosphorescence, Kasha's rule, Delayed fluorescence, Quantum yield, Mechanism and decay kinetics of photophysical processes. Fluorescence Quenching (dynamic and static), Stern Volmer equation. Energy transfer, Electron transfer phenomenon (Marcus theory, Rehm Weller theory), Proton transfer phenomenon, complex formation phenomenon (excimer, exciplex).

Module 2: Unit 1: Interaction of electromagnetic radiation with matter (8L)

Interaction of electromagnetic radiation with matter, Transition probabilities, Transition moment integral and its applications. Selection rules, Franck Condon principle, Oscillator strength, Nature of transitions, solvent effect on absorption and emission spectra, Stokes shift. Laser, different types and applications.

Module 3: Unit 3: Properties of electronically excited molecules and different non radiative electronic transition (8L)

Properties of electronically excited molecules: Life time,redox potential,dipole moment, pK values. Potential energy diagram for donor acceptor system, polarized luminescence.

Nonradiative intramolecular electronic transition; internal conversion, intersystem crossing, crossing of potential energy surface.

Module 4: Unit 3: Raman, Mossbauer, NQR and Photoelectron spectroscopy and applications (16L)

Raman Spectroscopy: Classical and quantum mechanical treatment of rotational and vibrational Raman spectra, Polarization and depolarization of Raman lines.Resonance Raman spectroscopy.

Mossbauer spectroscopy; Principles,technique,chemical shift,quadrupole effect,effects of magnetic field, applications. NQR spectroscopy: Principle, technique,coupling in atom, applications.

Photoelectron spectroscopy: principles and applications.

Text Books:

1. Lampman, G. M.; Pavia, D. L.; Kriz, G. S.; Vyvyan, J.R., *Introduction to Spectroscopy*, 5th Ed., Cengage Learning India, New Delhi (2015).
2. *An introduction to Photochemistry* by K.K.Rohatgi-Mukherjee.

Reference texts:

1. *Photochemistry* by Wayne and Wayne.
2. *Photochemistry* by J.A. Barltrop and J.D.Coyle
3. *Spectroscopy* by Raymond Chang
4. *Fundamentals of Molecular Spectroscopy* by C. N. Banwell
5. *Spectroscopy* by Barrow.
6. *Molecular Structure and Spectroscopy* by G.Aruldhas.
7. W. Kemp, *NMR in chemistry-A Multinuclear Introduction*, McMillan, 1986.

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcome (CO)	CO	PO
1	Photophysical processes in molecules	Module 1/Unit 1	20%	1. Changes in energy levels of a molecule after absorption of radiation can be learnt to understand the effect of sunlight on living systems.	CO1	PO1
2	Interaction of electromagnetic radiation with matter	Module 2/Unit 2	20%	2. Manufacture of laser can be learnt for use in different field.	CO2	PO2
3.	Properties of electronically excited molecules and different non radiative electronic transition	Module 3/Unit 3	20%	3. Life time in the excited states of molecules is known which helps in predicting the reactions at excited state.	CO3	PO1
4	Raman, Mossbauer, NQR and photoelectron spectroscopy and applications	Module 4/Unit 4	40%	4. Characterization of the molecules and their applications can be learnt for use in different field.	CO4	PO2

(Elective I) B. Cheminformatics

Paper code: MSAC304B
(3 Credit) (100 Marks)

Course Objectives:

1. To know how the information of a compound is stored in computer.
2. To find out a compound from a database using computer techniques.
3. To know the available softwere to draw chemical structure of compounds.
4. To know the important properties of a compound to be a drug.
5. To know different methods to design a drug.

Module 1: Unit-1: In-silico Representation of Chemical Information **(10L)**

a. CIF IUCr Crystallographic Information Framework
b. CML Chemical Markup Language
c. SMILES -- Simplified Molecular Input Line Entry Specification
d. Graph theory and its application
e. InChi -- IUPAC International Chemical Identifier
f. Other representations

Module 2: Unit-2: Chemical Databases and Data Mining **(10L)**

a. Cambridge Structural Database CCDC CSD
b. Crystallographic Open Database COD
c. Protein Data Bank PDB Ligand Explorer
d. Chemspider
e. Other Data Bases

Module 3: Unit-3: Molecular Drawing and Interactive Visualization **(10L)**

a. ChemDraw
b. Marvin Sketch
c. ORTEP
d. Chimera, RasMol, PyMol
e. Quantumwise

Module 4: Unit-4: Computer-Aided Drug Design Tools **(10L)**

a. Molecular Modelling Tools
b. Structural Homology Modelling Tools
c. Docking Tools and Screening Tools
d. Methods for computation of IC_{50}, LogP, toxicity etc.

Text books:

1. *Chemoinformatics: A Textbook*, Johann Gasteiger (Editor), Thomas Engel (Editor), November 2003, Wiley.
2. *Chemoinformatics in Drug Discovery*, Tudor I. Oprea (Editor), Raimund Mannhold (Series Editor), Hugo Kubinyi (Series Editor), Gerd Folkers (Series Editor), March 2006, Wiley.

Reference texts:

1. *Chemoinformatics in Drug Discovery*, Prof. Dr. Tudor I. Oprea, 26 January, 2005. Wiley online library.

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcome (CO)	CO	PO
1.	In-silico Representation of Chemical Information	Module 1/Unit 1	10	1.Will be able to identify a compound written in different format.	CO1	PO2
2.	Chemical Databases and Data Mining	Module 2/Unit 2	20	2.Will be able to search drug like compounds from a data base to test new compounds as a drug.	CO2	PO2
3.	Molecular Drawing and Interactive Visualization	Module 3/Unit 3	10	3.Will be able to draw and store a compound in computer.	CO3	PO2
4.	Computer-Aided Drug Design Tools	Module 4/Unit 4	30	4.Will be familiar with the different properties of a drug.	CO4	PO3
5.	Computer-Aided Drug Design Tools	Module 4/Unit 4	30	5.Will be able to design a drug and predict its drug efficacy.	CO5	PO3

(Elective I) C. Water and Wastewater Treatment **Paper code:MSAC304C**
(3 Credit) (100 Marks)

(Elective I) D. Semiconductor devices **Paper code:MSAC304D**
(3 Credit) (100 Marks)

(Elective II) A. Colloids, Surface chemistry, Catalysis and Solid state

Paper code: MSAC305A

(3 Credit) (100 Marks)

Course Objectives:

1. Colloidal solution can be prepared and can be classified according to their properties.
2. Adsorption techniques may be used to understand complicated reactions and can be used for purification process.
3. Catalysysts have been classified and importance of them to any reaction can be understood for application in industrial processes.
4. Properties of solids have been described for their application in electronic industry.

Module 1: Unit 1: Colloids **(8L)**

Preparation, properties, stability and application of colloids.

Module 2: Unit 2: Surface chemistry **(10L)**

Introduction, Difference between adsorption and absorption, Types of adsorption - Adsorption isotherm-Freundlich Adsorption Isotherms, Langmuir Adsorption Isotherm, Gibbs adsorption isotherm, BET equation, Harkins Jura equation-Surface Films, Micelles, microemulsion.

Module 3: Unit 3: Catalysis and applications **(10L)**

Different type of catalysts and their characteristics. Homogeneous Catalysis, Heterogeneous Catalysis. Mechanism of Catalytic Reaction. Kinetics of Surface Reaction, Kinetics of Bimolecular Reaction (Langmuir-Hinshelwood), Catalytic Poisoning and Promoters Application of Catalysis, Enzymes. Kinetics of Enzyme Catalysed Reaction or Michaelis and Menten equation, Factors Affecting Enzyme Activity.

Module 4: Unit 4: Solid State **(8L)**

Crystal structures; Bragg's law and applications; band structure of solids. Defects of crystal, Computational approach for periodic calculations, density of states and band structure.

Text Books:

1. Physical Chemistry by G.W.Castellan
2. Physical Chemistry by S.Glasstone

Reference texts:

1. Physical Chemistry by I.N.Levine
2. Physical Chemistry by Dr. S. Pahari
3. Micellar Catalysis by Fendler and Fendler.
4. Physical Chemistry by Walter J. Moore.

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcome (CO)	CO	PO
1	Colloids, Preparation and Properties	Module 1/Unit 1	20%	1.Purification of water can be done by formation of colloids. Solubilisation of material can be done.	CO1	PO1
2	Adsorption phenomenon and applications	Module 2/Unit 2	30%	2.Different resins can be produced applying adsorption technique for softening of water to be used in industry	CO2	PO3
3.	Catalysis and	Module	30%	3.Different catalysts can be	CO3	PO2

	applications	3/Unit 3		identified according to the needs in industry for fruitful applications.		
4.	Crystal structure, defects, density of states	Module 4/Unit 4	20%	4.Semiconductors of different types can be made according to need in electronic industry.	CO4	PO3

(Elective II) B. Industrial Chemistry

Paper code: MSAC305B
(3 Credit)(100 Marks)

Course Objectives:

1. Basic principles of different separation processes.
2. Preparation of gases and chemicals for industrial use.
3. Manufacture of chemicals of industrial importance.
4. Metallurgy and Ceramics

Module 1: Unit -1: Chemical Technology (10L)

Basic principles of distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, separation by absorption and adsorption. An introduction into the scope of different types of equipment needed in chemical technology, including reactors, distillation columns, extruders, pumps, mills, emulgators. Scaling up operations in chemical industry. Introduction to clean technology.

Module 2: Unit -2: Industrial Gases and Inorganic Chemicals (10L)

Industrial Gases: Large scale production, uses, storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, sulphur dioxide and phosgene. Oils and waxes. Polymer – plastic, rubber.

Module 3: Unit -3: Inorganic Chemicals (10L)

Inorganic Chemicals: Manufacture, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, common salt, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate and potassium permanganate. Soap and detergent. Fertilizer. Glasses. Cement.

Module 4: Unit -4: Industrial Metallurgy and Ceramics (10L)

Preparation of metals (ferrous and non-ferrous) and ultra-pure metals for semiconductor technology. Crystalline ceramics and Noncrystalline ceramics and their electrical and optical properties.

Text books:

1. ULLMANN's Encyclipedia of Industrial Chemistry
2. Industrial chemistry: Part 1 & part 2: by R. K. das

Refernce texts:

1. Dryden's outlines of Chemical Technology for 21st Century by Kirk-Othmer.
2. Industrial Inorganic chemistry by Mark Anthony Benvenuto.

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcome (CO)	CO	PO
1	Chemical technology	Module 1/Unit 1	25%	1. Separation of components from a mixture will be learnt, for scaling up operations in chemical industries	CO1	PO3
2	Industrial gases and inorganic chemicals	Module 2/Unit 2	25%	2. To acquire knowledge in large-scale production of industrial gases for application in Industry	CO2	PO3
3	Inorganic chemicals	Module 3/Unit 3	25%	3. To gain knowledge about different chemical manufacturing for use as raw material in industrial processes	CO3	PO3

4	Industrial metallurgy and ceramics	Module 4/Unit 4	25%	4. To learn extraction of metals and preparation of pure metals of use in semi-conductor and ceramic technology	CO4	PO3

(Elective II) C. Sensor Development

Paper code:MSAC305C
(3 Credit)(100 Marks)

(Elective II) D. Solid Waste Management and Air Pollution

Paper code: MSAC305D
(3 Credit)(100 Marks)

Computer Programming-II

Paper code:MSAC391
(2 Credit)(100 Marks)

(20hr)

Course Objectives:

1. To know how to ues different Computational Chemistry packages to solve chemical problems.
2. To know how to write efficient computer program to solve chemical problem.
3. To know to write interface programs for data analysis.

Module 1: Unit-1: Electronic structure and property problem **(10Hr)**
Solving of chemical problem using Computational Chemistry packages like GAMESS, Gaussian, Quantum Expresso, NWchem

Module 2: Unit-2: Molecular Dynamic Simulation **(10Hr)**
Solving of dynamic properties of a chemical system using Molecular Dynamic Simulation. (Different online or off line packages may be used for practice)

References Texts:

1.GAMESS manual
2.Gaussian manual
3. *The Art of Molecular Dynamics Simulation - by D.C. Rapaport*

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcome (CO)	CO	PO
1	Electronic structure and property problem	Module 1/Unit-1	60%	1.Will be able to compute electronic structure and properties of a chemical system.	CO1	PO2
2	Molecular Dynamic Simulation	Module 2/Unit-2	40%	1.Will be able to compute dynamical properties of a chemical system	CO2	PO2

Preparation of complex materials and their characterization by physiochemical techniques

Paper code:MSAC392
(3 Credit) (100 Marks)

(40hr)

Course Objectives:

1. To determine relative average molecular mass of a polymer by viscosity method.
2. To determine thermodynamic solubility product of a sparingly soluble salt in aqueous medium.
3. To perform conductometric titration of a mixture of HCl and CH_3COOH with NaOH.
4. To determine CMC of surfactants from interfacial tension measurements.
5. To determine rate constant of acid catalysed inversion of canesugar by polarimetric method.
6. To determine second order rate constant of alkaline hydrolysis of ester by conductometric method.
7. To perform potentiometric titration of Ferrous ion by dichromate and evaluation of the formal potential of Fe^{3+}/Fe^{2+}.
8. To determine the redox potential E^0 of the quinhydrone electrode by potentiometric method and pH of buffer solution.

Module 1: Unit 1:

1. Determination of relative average molecular mass of a polymer by viscosity method.
2. Determination of thermodynamic solubility product of a sparingly soluble salt in aqueous medium.

Module 2: Unit 2:

1. Conductometric titration of a mixture of HCl and CH_3COOH with NaOH.
2. Determination of CMC of surfactants from interfacial tension measurements.

Module 3: Unit 3:

1. Determination of rate constant of acid catalysed inversion of canesugar by polarimetric method.
2. Determination of second order rate constant of alkaline hydrolysis of ester by conductometric method.

Module 4: Unit 4:

1. Potentiometric titration of Ferrous ion by dichromate and evaluation of the formal potential of Fe^{3+}/Fe^{2+}.
2. Determination of the redox potential E^0 of the quinhydrone electrode by potentiometric method and pH of buffer solution.

Reference texts:

1. *Practical Physical Chemistry* by S.R.Palit and A.K.De.
2. *Experimental Physical Chemistry* by V.D.Athawale and Parul Mathur.

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcome (CO)	CO	PO
1	Determination of relative average molecular mass of a polymer by viscosity method. Determination of thermodynamic solubility product of a sparingly soluble salt in aqueous medium	Module-1	25	1.Characterization of molecules can be done for their applications	CO1	PO2
2	Conductometric titration of a mixture of HCl and CH_3COOH with NaOH. Determination of CMC of surfactants from interfacial tension measurements.	Module-2	25	2.Estimation of the components amount in a mixture.	CO2	PO2
3	Determination of rate constant of acid catalysed inversion of canesugar by polarimetric method. Determination of second order rate constant of alkaline hydrolysis of ester by conductometric method.	Module-3	25	3.Rate of reactions are known for applications.	CO3	PO2
4	Potentiometric titration of Ferrous ion by dichromate and evaluation of the formal potential of Fe^{3+}/Fe^{2+}. Determination of the redox potential E_0 of the quinhydrone electrode by potentiometric method and pH of buffer solution.	Module-4	25	4.Characterization of electrodes are done.	CO4	PO2

Spectrpscopic Analysis Lab

Paper code:MSAC393
(3 Credit)(100 Marks)

Spectroscopic Analysis: (40hr)

1. Determination of bonding in a molecule by using Fourier Transform Infrared (FTIR) spectroscopy.
2. Characterization of an compound by Attenuated Total Reflection Infra-Red Spectroscopy (ATR-FTIR, MID-IR).
3. Study of a charge-transfer complex between iodine and tritron-X 100 using UV-visible Spectroscopy (UV-Vis).
4. Determination of bond length of a diatomic molecule by Far-Infra-Red and Near Infra-Red spectroscopy.
5. Study of protein folding and defolding by Circular Dichroism (CD), and ORD.
6. Estimation of quenching constant of fluorescence quenching of a fluorescent molecule by Fluorescence spectrophotometer.
7. Quenching of fluorescence of a fluorescent molecule will be studied by time resolve fluorescence spectrophotometer.
8. Analysis and interpretation of sample data of given chemicals or compounds using Origin/ ChemOffice softwares.

Project-III

Paper code: MSAC394
(3 Credit)(100 Marks)

Students will be offered different research topics according to their choice which will be reviewed, analysed and a report needs to submitted to the concerned departmental faculty before the start of semester III examination. A presentation will be made and delivered in presence of the departmental faculty members for assessment.

SEMESTER – IV

(Elective III) A. Pharmaceutical Chemistry

Paper code:MSAC401A
(3 Credit) (100 Marks)

Course Objectives:

1. To handle doctor's prescription.
2. To know about how to prepare different medical solutions.
3. To know about different types of powder used in medicinal techniques.
4. To know how drugs act in our body.
5. To know how the dose of a drug is considered.
6. To know what is the process after the action of a drug.

Module 1: Unit-1: Pharmaceutics basics **(15L)**

a. ***Prescription:*** Parts of prescription, handling of prescription, Posology.
b. ***Solution:*** Formulation, aqueous and non-aqueous vehicles, factors affecting rate of solubilization and solubility, methods to improve aqueous solubility, formulation additives; Elixirs; Linctus; Mouthwashes and Gargles; Nasal and Ear drops; Lotions; Stability of solution; Syrups.
c. ***Powder:*** Classification, advantages of powder formulation, milling, mixing and dividing of powders, factors influencing blending of powders, powders containing liquids, eutaxia.
d. Pharmaceutical calculations Labelling of Pharmaceutical products

Module 2: Unit -2: Basics of Drug Action **(25L)**

a. ***Interactions:*** Inter- and intramolecular interactions. Weak interactions in drug molecules. Chirality and drug action. Covalent, ion-ion, ion-dipole, Hydrogen bonding, C-H hydrogen bonding, dihydrogen bonding, Van der Waals interactions and the associated energies
b. ***Receptorology:*** Drug-receptor interactions, Receptor theories and drug action: Occupancy Theory, Rate Theory, Induced Fit Theory, Macromolecular perturbation theory, ActivationAggregation theory. Topological and stereochemical consideration.
c. ***Enzyme Kinetics:*** enzyme kinetics in drug action. Do all molecules of an enzyme have same kinetics? Mechanisms of enzyme catalysis, Electrostatic catalysis and desolvation. Covalent catalysis, Acid-base catalysis, Strain / distortion in enzyme catalysis. Coenzyme catalysis.
d. ***Enzyme Inhibition***: Drug action through enzyme inhibition. Examples based on PDE4, GSK3, etc. Theories of enzyme inhibition and inactivation. Enzyme activation of drugs prodrugs.
e. ***Nucleic acids& drug research:*** NA as targets for drug action. NA-interactive agents. Classes of drugs that interact with nucleic acids. Intercalation, NA-alkylation, NA-strand breaking and their importance in drug action.
f. ***Drug likeness:*** Drug like molecules and theories associated with the recognition of drug like properties. Physical organic chemistry of Drug metabolism, drug deactivation and elimination.
g. ***Drug action after Metabolism:*** Phase I and Phase II transform.Concept of hard and soft drugs. Chemistry of ADME and Toxicity properties of drugs.

Text books:

1. C.O. Wilson, J.M. Beale, J.H. Block, *Textbook of Organic Medicinal and Pharmaceutical Chemistry*, 12th Edn., Lippincott Williams and Wilkins, 2010.
2. J. P. Remington, *Remington's Pharmaceutical Sciences*, Vol.13, 19th Edn., Mack, 1990.

Reference texts:

1. *Pharmaceutical Chemistry – I*, Dr. A. V. Kasture, Dr Sg Wadodkar, Pragati Books Pvt. Ltd., 2015
2. *Essentials of Pharmaceutical Chemistry*, Cairns, Donald, Fourth edition, 2012

3. *A Textbook of Pharmaceutical Chemistry*, Jayashree Ghosh, S. Chand Publishing, 2010.

Sl. No.	Content of the course	Module No.	%age of questions	Course Outcome (CO)	CO	PO
1.	Pharmaceutics basics	Module 1/Unit-1	5	1.Will be able to explain the prescription of a doctor.	CO1	PO3
2.	Pharmaceutics basics	Module 1/Unit-1	15	2.Will be able to learn the variation of solutions used in medicine.	CO2	PO3
3.	Pharmaceutics basics	Module 1/Unit-1	15	3.Will be able to prepare and identify different types of powder used to prepare medicine.	CO3	PO3
4.	Basics of Drug Action	Module 2/Unit-2	15	4.Will be able to know how drugs works in our body.	CO4	PO1
5.	Basics of Drug Action	Module 2/Unit-2	25	5.Will be able to know about the importance and measurement methods of IC_{50} of a drug.	CO5	PO1
6.	Basics of Drug Action	Module 2/Unit-2	25	6.Will be able to know different process of the metabolism of a drug.	CO6	PO1

(Elective III) B. Food Chemistry

Paper code: MSAC401B
(3 Credit) (100 Marks)

(Elective III) C. Industrial Catalysis

Paper code: MSAC401C
(3 Credit) (100 Marks)

(Elective III) D. Industrial & Environmental Pollution Management and Industrial Process Safety

Paper code: MSAC401D
(3 Credit) (100 Marks)

Industrial Exposure

Paper code: MSAC491
(2 Credit)(100 Marks)

To visit industry facility and subsequent submission of a report to the department from individual student. This is a value added course for students. Credits may be transferred after submission of report.
For industrial exposure, any industry should be chosen for the visit to observe their work and the experience in report form shall have to be submitted to the department.

Project -IV (Dissertation & Viva-voce)

Paper code:MSAC492
(12 Credit) (100 Marks)

1. Review of literature, project work and submission of dissertation.
2. Viva-voce on submitted work.

Laboratory work on any topic which will be useful for further studies, to be performed in-house or in any institute. After completion of work of minimum 12 weeks duration the project report shall be submitted in dissertation form before semester IV exam and that will be evaluated after the theory exam through presentation on submitted work followed by viva-voce in presence of a committee constituted by an external expert and internal teachers.