Shri Rawatpura Sarkar University, Raipur

Examination Scheme & Syllabus

for

Two Year Master of Science in Chemistry Programme

M.Sc. Chemistry Semester-I

(Effective from the session: 2022-2023)

Shri Rawatpura Sarkar University
Raipur, Chhattisgarh
Faculty of Science
Department of Chemistry
Two Year Master of Science in Chemistry Programme
M.Sc. Chemistry Semester-I
Scheme of Teaching and Examination

Outcome Based Education (OBC) and Choice Based Credit System (CBCS)
(Effective from the session: 2022-2023)

S. No.	Course Code	Course Title	Hours/ Week			Credit	Maximum Marks			Sem End Exam Duration (Hrs)
			L	T	P		Continuation Evaluation	Semester End Examination	Total	
1	SMS04101T	Inorganic chemistry I:Chemistry of metal complexes and Group Theory	4	-	-	4	30	70	100	3.0
2	SMS04102T	Organic Chemistry I: Concept in organic chemistry	4	-	-	4	30	70	100	3.0
3	SMS04103T	Physical Chemistry I: Quantum chemistry, Thermodynamics and chemical dynamics-I and surface chemistry	4	-	-	4	30	70	100	3.0
4	SMS04104T	Theory and Application of Spectroscopy I	4	-	-	4	30	70	100	3.0
5	SMS04181P	Chemistry Lab course: I	-	-	4	2	-	-	50	5.0
6	SMS04182P	Chemistry Lab Course: II	-	-	4	2	-	-	50	5.0
7	SMS04121T	Computer Application and Chemoinformatics	2	-	-	2	15	35	50	2.0
	Total teaching hrs/week: 26		**Total Credits**			**22**	**Total Marks**		550	

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<table>
<tr><td>Course Title</td><td colspan="5">INORGANIC CHEMISTRY I: Chemistry of metal complexes and Group Theory</td></tr>
<tr><td>Course Code</td><td colspan="5">SMS04101T</td></tr>
<tr><td rowspan="2">Course Credit</td><td>L</td><td>T</td><td>P</td><td>TC</td><td></td></tr>
<tr><td>4</td><td>-</td><td>-</td><td>4</td><td></td></tr>
<tr><td>Prerequisite</td><td colspan="5">Students must have the knowledge of periodic properties of elements and their application.</td></tr>
<tr><td>Course Objective</td><td colspan="5">• Inorganic Chemistry in advance and establish foundation to research in the respective domain.</td></tr>
<tr><td>Content</td><td colspan="5">UNIT-I
Stereochemistry and Bonding in Main Group Compounds: VSEPR, Walsh diagram (triatomic and penta-atomic molecules), dribonds, bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules, Metal-Ligand: Equilibrium in solution stepwise and overall formation constants and their interaction, trends in stepwise constant, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand. Chelate effect and its thermodynamic origin, determination of binary formation constants by potentiometry and spectrophotometry.
UNIT-II
Metal-Ligand bonding Limitation of crystal field theory, molecular orbital theory for bonding in octahedral, tetrahedral and square planar complexes, π-bonding and molecular orbital theory, Metal –Complexes: Metal carbonyl, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding structure and important reaction of transition metal nitrosyl, dinitrogen and dioxgen complexes; tertiary phosphine as ligand.
UNIT-III
Isopoly and heteropoly acid: Isopoly and heteropoly acids of Mo and W. Preparation, properties and structure. Classification, Preparation, properties and structures of borides, carbides, nitrides and silicides, Silicates- classification and Structure, Silicones- preparation, properties and application.
UNIT- IV
Metal Clusters: Higher boranes, carboranes, metalloboranes and metallo-carboranes compounds with metal metal multiple bonds. Crown ether complexs and cryptands, inclusion compounds, Chains: catenation, heterocatenation, intercatenation. Rings: Borazines, phosphazines.
UNIT V
Symmetry and Group theory in Chemistry:Symmetry elements and symmetry</td></tr>
</table>

	operation, definition of group, subgroup., reaction between orders of a finite group and its sub-group, Conjugacy relation and classes. Point symmetry group. Schonfilies symbols, representations of groups by matrices (representation for the Cn, Cnv, Cnh, Dnh group to be worked out explicity). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy.
Course Outcome	• On the completion of this course successfully student will be able to understand the development of the inorganic chemistry.
Text Books	1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley. 2. Inorganic Chemistry, J.E. Huhey, Harpes and Row. 3. Chemistry of the Elements, N.N. Greenwood and A. Earnshow, Pergamon. 4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier. 5. Comprehensive Coordination Chemistry Eds. G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.
Reference Books	1. Magnetiochemistry, R.1. Carlin, Springer Verlag. 2. Comprehensive Coordiantion Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon. 3. Advance Inorganic Chemistry, S. K. Agrawal & K. Lal, Pragati Prakashan

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<table>
<tr><td>Course Title</td><td colspan="5">ORGANIC CHEMISTRY I: Concept in organic chemistry and photochemistry</td></tr>
<tr><td>Course Code</td><td colspan="5">SMS04102T</td></tr>
<tr><td rowspan="2">Course Credit</td><td>L</td><td>T</td><td>P</td><td>TC</td><td></td></tr>
<tr><td>4</td><td>-</td><td>-</td><td>4</td><td></td></tr>
<tr><td>Prerequisite</td><td colspan="5">Students must have the knowledge of nomenclature and isomerism of organic molecules</td></tr>
<tr><td>Course Objective</td><td colspan="5">• Organic Chemistry in advance and establish foundation to research in the respective domain.</td></tr>
<tr><td>Course Content</td><td colspan="5">UNIT-I
Nature of Bonding in Organic Molecules: Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerences, tautomerism, Aromaticity: Aromacity in benzenoid and non-benzoid compounds, alternate and non-alternate hydrocarbons. Huckel’s rule, energy. Level of π-molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent-addition compounds,
UNIT-II
Conformational: analysis of cycloalkanes, decalins, effect of confirmation of reactivity, confirmation of sugars, steric strain due to unavoidable crowding ,Stereochemistry: Elements of symmetry, chirality, molecules with more than one chiral center, threo and ertythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereo selective synthesis, Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spirane chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.
UNIT -III
Reaction intermediates: Generation, structure, stability and reactivity of carbocation~carbanions, free radicals, carbenes, Nitrenes, and Benzynes. Application of NMR in detection of carbocations, Free Radical Reactions: Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboyxlic acids, autooxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, sandmeyer reaction, free radical rearrangement andhunsdiecker reaction.
UNIT-IV
Pericyclic Reactions: Molecular orbital symmetry, frontier orbitals of ethylene,</td></tr>
</table>

	1,3-butadiene, 1,3,5hexatriene and allyl system. Classification of periycyclic reactions, woodward-hoffmann correlation diagrams, FMO and PMO approach. Electrocyclic reactions-conrotatory and disrotatory motions, 4n 4n+2 and allyl systems. Cycloadditions-antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotrpic reactions. Sigmatropic rearrangements-suprafacial and antarafacial shifts of H, sigmatropic involving carbon moieties, 3,3- and 5,5 sigmatropic rearrangements, claisen, cope and aza-cope rearrangements, fluxional tautomerism and enereaction. **UNIT -V** **Photochemical Reactions:-**Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum field, transfer of excitation energy, actinometry, Determination of Reaction Mechanism Classification, rate constants and life times of reactive energy state determination of rate constants of reactions, Effect of light intensity on the rate of photochemical reactions, Types of photochemical reactions-photo dissociation, gas-phase photolysis, Miscellaneous Photochemical Reactions:- Photo-Fries reactions of annelids, Photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen and its reactions, Photo-chemical formation of smog, Photo-degration of polymers, Photochemistry of vision, Photo chemistry of Aromatic Compounds- Isomerisations, additions and substitutions
Course Outcome	• On the completion of this course successfully student will be able to understand the development of the organic chemistry.
Text Books	1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley. 2. Advanced Organic Chemistry, F.A. Carey and R.J. Sunderg, Plenum. 3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman. 4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Comell University Press. 5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall. 6. Modern Organic Reactions, H.O. House, Benjamin.
Reference Books	1. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic &Professionsl. 2. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan. 3. Pericyclic Reactions, S.M. Mukherji, Macmillan, India 4. Stereochemistry of Organic Compounds, D.Nasipuri, New Age International. 5. Stereochemisty of Organic Compounds, P.S. Kalsi, New Age International

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M.Sc. Chemistry Semester-I
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<table>
<tr><td>Course Title</td><td colspan="5">PHYSICAL CHEMISTRY I: Quantum chemistry, Thermodynamics and chemical dynamics-I and surface chemistry</td></tr>
<tr><td>Course Code</td><td colspan="5">SMS04103T</td></tr>
<tr><td rowspan="2">Course Credit</td><td>L</td><td>T</td><td>P</td><td>TC</td><td></td></tr>
<tr><td>4</td><td>-</td><td>-</td><td>4</td><td></td></tr>
<tr><td>Prerequisite</td><td colspan="5">Students must have the basic knowledge of general physical chemistry and calculus.</td></tr>
<tr><td>Course Objective</td><td colspan="5">• Physical Chemistry in advance and establish foundation to research in the respective domain.</td></tr>
<tr><td>Course Content</td><td colspan="5">UNIT-I
Introduction to Exact Quantum Mechanical: Results The Schrödinger equation and the postulates of quantum mechanics. Discussion of solutions of the schrödinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom and helium atom. Approximate Methods: The variation theorem, linear variation principle. Perturbation theory (First order and nondegenerate). Applications of variation method and perturbation theory to the helium atom.
UNIT-II
Classical Thermodynamics: Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar free energy, partial molar volume and partial molar heat content and their significance. Determinations of these quantities. Concept of fugacity and determination of fugacity. Non-ideal systems: Excess function s for non-ideal solutions, activity, activity coefficient, debyehuckel theory for activity coefficient of electrolytic solutions, determination of activity and activity coefficients, ionic strength. Application of phase rule.
UNIT-III
Chemical Dynamics I: Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogenbromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousov -Zhabotinsky reaction).
UNIT-V
Electrochemistry I: Electrochemistry of solutions. Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Debye-Huckel-Jerum mode.</td></tr>
</table>

	Thermodynamics of electrified interface equations. Derivation of electro capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Guoy-Chapman, Stern, Graham-Devanathan-Mottwatts, Tobin, Bockris, Devanlhan models. Overpotentials, exchange current density, derivation of Butler Volmer equation, Tafel plot. Quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling **UNIT-V** **Adsorption:** Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), Surface films on liquids (Electro-kinetic phenomenon) catalytic activity at surface. Micelles: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solublization, micro emulsion, reverse micelles.
Course Outcome	• On the completion of this course successfully student will be able to understand the development of the physical Chemistry.
Text Books	1. Physical Chemistry, P.W. Atkins, ELBS. 2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill. 3. Quantum Chemistry, Ira N. Levine, Prentice Hall. 4. Coulson's Valence, R.McWeen y, ELBS. 5. Chemical Kinetics. K.J. Laidler, McGraw-Hill.
Reference Books	1. Kinetics and Mechanism of Chemical Transformation J.Rajaraman and J. Kuriacose, McMillan. 2. Micelles, Theoretical and Applied Aspects, V. MOraoi, Plenum. 3. Modern Electrochemistry Vol. 1 and Vol II J.O.M. Bockris and A.K.N. Reddy, Planum. 4. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.

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2022-2023

<table>
<tr><td>Course Title</td><td colspan="5">THEORY AND APPLICATION OF SPECTROSCOPY: I</td></tr>
<tr><td>Course Code</td><td colspan="5">SMS04104T</td></tr>
<tr><td rowspan="2">Course Credit</td><td>L</td><td>T</td><td>P</td><td>TC</td><td></td></tr>
<tr><td>4</td><td>-</td><td>-</td><td>4</td><td></td></tr>
<tr><td>Prerequisite</td><td colspan="5">Students must have the knowledge of interaction between light and matter and quantum mechanics.</td></tr>
<tr><td>Course Objective</td><td colspan="5">• Spectroscopy Chemistry in advance and establish foundation to research in the respective domain.</td></tr>
<tr><td>Course Content</td><td colspan="5">UNIT -I
Unifying Principles: Electromagnetic radiation, interaction of electromagnetic radiation with matter absorption, emission transmission, reflection, dispersion, polarization and scattering, Uncertainty relation and natural line width and natural line broadening, transition probability, selection rules, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels.
UNIT -II
Microwave Spectroscopy: Classification of molecules in term of their internal rotation mechanism, determination of rotation energy of diatomic and polyatomic molecules, intensities of rotational spectral lined, effect of isotopic substitution on diatomic and polyatomic molecules, intensities of rotational spectral lines and parameters of rotational energy of linear and the transition frequencies, non-rigid rotators, spectral lines and parameters of rotational energy of linear and symmetric top polyatomic molecules. Application in determination of bond length.
UNIT- III
Scattering Spectroscopy:-Principle, instrumentations and application of Auger spectroscopy and Scanning Electron Microscopy for chemical characterization, electron diffraction of gases and vapours, The Wierl equation and co- related method, application of electron diffraction. Theory, instrumentation and application of turbidimetry, nephelometry and fluorometry. Fluoroscence and phosphorescence and factors affecting them.
UNIT -IV
Raman Spectroscopy:-Classical and quantum theories of Raman effect, pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules mutual exclusion principle, Resonance Raman spectroscopy, Coherent anti Stokes Raman spectroscopy (CARS), Instrumentation , Application of Raman effect in molecular-structures, Raman activity of molecular vibration, structure of CO_2, N_2O, SO_2, NO_3 , CIF_3</td></tr>
</table>

	UNIT -V **X-ray Diffraction:** Bragg condition, Miller indices, Laue Method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern, Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramcharan diagram. **Electron Diffraction:** Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces. **Neutron Diffraction :** Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.
Course Outcome	• On the completion of this course successfully student will be able to understand the development of the spectroscopy.
Text Books	1. Modern Spectroscopy, J.M. Hollas, John Viley. 2. Applied Electron Spectroscopy for chemical analysis d. H. Windawi and F.L. Ho, Wiley Interscience. 3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood. 4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
Reference Books	1. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill. 2. Basic Principles of Spectroscopy, R. Chang, McGraw Hill. 3. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH Oxford. 4. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley. 5. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, harper & Row.

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M.Sc. Chemistry Semester-I
2022-2023

<table>
<tr><td>Course Title</td><td colspan="5">CHEMISTRY LAB COURSE:I</td></tr>
<tr><td>Course Code</td><td colspan="5">SMS04181P</td></tr>
<tr><td rowspan="2">Course Credit</td><td>L</td><td>T</td><td>P</td><td>TC</td><td></td></tr>
<tr><td>-</td><td>-</td><td>2</td><td>2</td><td></td></tr>
<tr><td>Prerequisite</td><td colspan="5">Students must have the practical knowledge of chemical analysis for inorganic and organic molecules.</td></tr>
<tr><td>Course Objective</td><td colspan="5">• To understand the practical concepts of inorganic and organic chemistry</td></tr>
<tr><td>Course Content</td><td colspan="5">A. Inorganic Chemistry
1. Qualitative analysis of mixture containing eight radical including two less common metal from among the following by semi micro method. Basic Radicals : Ag, Pb, Hg, Bi, Cu, Cd, As, Sb, Sn, Fe, Al, Cr, Zn, Mn, Co, Ni, Ba, Sr, Ca, Mg, Na, K, Ce, Th, Zr, W, Te, Ti, Mo, U, V, Be, Li, Au, Pt. Acid Radicals :Carbonate, Sulphite, Sulphide, Nitrite, Nitrate, Acetate, Flouride. Chloride, Bromide, Iodide, Sulphate, Borate, Oxalate, Phosphate, Silicate, Thiosulphate, Ferrocyanide, Ferricyanide, Sulphocyanide, Chromate, Arsenate and Permanganate.
2. Quantitative analysis: Involving separation of two of the following in ores, alloys, or mixtures in solution, one by volumetric and the other by gravimetric methods.
3. Estimation of :
a. Phosphoric acid in commercial orthophosphoric acid.
b. Boric acid in borax.
c. Ammonia in a ammonium salt.
d. Manganese dioxide in pyrolusite.
e. Available chlorine in bleaching powder.
f. Hydrogen peroxide in commercial samples.
4. Preprations: Preparation of selected inorganic compound and their studies by I.R. electronic spectra, Mössbauer, E.S.R. and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds
a. $VO(acac)_2$
b. $TiO(C_9H_8NO)_2 . 2H_2O$
c. cis-K $[Cr(C_2O_4)_2 (H_2O)_2]$
d. Na $[Cr (NH_3)_2 (SCN)_4]$</td></tr>
</table>

	e. $Mn(acac)_3$ f. $K_2[Fe(C_2O_4)_3]$ g. Prussian Blue, Turnbull's Blue. h. $[Co(NH_3)_6]$ $[Co(NO_2)_6]$ i. cis-$[Co(trien)(NO_2)_2]$ $Cl.H_2O$ j. $Hg[Co(SCN)_4]$ k. $[Co(Py)_2Cl_2]$ l. $[Ni(NH_3)_6]Cl_2$ m. $Ni(dmg)_2$ n. $[Cu(NH_3)_4]SO_4.H_2O$ 5. Detection of elements (N, Cl, S) by Lassaigne's test 6. Detection of the following functional groups by systematic chemical analysis: Aromatic amino ($-NH_2$), aromatic nitro ($-NO_2$), Aimdo ($-CONH_2$, including imide), Phenolic –OH, Carboxylic acid (-COOH), Carbonyl (>C=O); only one test for each functional group is to be reported.
Course Outcome	• On the completion of this course successfully student will be able to understand practical of inorganic chemistry and organic chemistry. .
Text Books	1. Vogel's Textbook of Quantitative Analysis, revi Mendham, ELBS. 2. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly, Prentice Hall. 3. Practical Organic chemistry by A. I. Vogel. 4. Practical Organic chemistry by Mann and Saunders. 5. Practical Organic chemistry by Garg and Salija.
Reference Books	1. The Systematic Identification of Organic compounds, R. L. Shriner and D. Y. Curtin. 2. Semimicro Qualitative Organic Analysis, N.D. Cheronis, J. B. Entrikin and E. M. Hodnett. 3. Practical Physical chemistry by Alexander Findlay. 4. Experimental Physical chemistry, D. P. Shoemaker, G. W. Garland and J. W. Niber, McGraw Hill Interscience. 5. Findlay's Practical Physical chemistry, revised B

Two year Master of Science in Chemistry programme
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2022-2023

<table>
<tr><td>Course Title</td><td colspan="5">CHEMISTRY LAB COURSE:II</td></tr>
<tr><td>Course Code</td><td colspan="5">SMS04182P</td></tr>
<tr><td rowspan="2">Course Credit</td><td>L</td><td>T</td><td>P</td><td>TC</td><td></td></tr>
<tr><td>-</td><td>-</td><td>2</td><td>2</td><td></td></tr>
<tr><td>Prerequisite</td><td colspan="5">Students must have the practical knowledge of handling spectroscopy and physical chemistry experiment.</td></tr>
<tr><td>Course Objective</td><td colspan="5">• To understand the practical concepts of spectroscopy and physical chemistry</td></tr>
<tr><td>Course Content</td><td colspan="5">1. Adsorption/Surface chemistry
a. To Study Surface Tension - Concentration relationship for solutions (Gibbs equation).
b. To Verify the Freundlich and Langmuir Adsorption isotherms using acetic acid/Oxalic acid and activated charcoal.
c. Determination of CMC of surfactants.
2. Phase equilibria
a. To Construct the Phase diagram for three component system (e.g., chloroform-acetic acid-water).
3. Chemical kinetics
a. Determination of the effect of (i) Change of temperature (ii) Change of concentration of reactants and catalyst and (iii) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.
b. Determination of the velocity constant of hydrolysis of an ester/ionic reaction in micellar media.
c. Determination of the rate constant for the decomposition of hydrogen peroxide by Fe+++ and Cu++ ions.
d. Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion).
4. Solutions/molecular weights
a. Determination of molecular weight of non-volatile substances by Landsber
b. Determination of molar masses of Naphthelene/acetanilide
c. Molecular weight of polymers by viscosity measurements.</td></tr>
</table>

	5. Conductometry a. Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically. b. Determination of solubility and solubility product of sparingly soluble salts (e.g., PbSO4, BaSO4) conductometrically. c. Determination of pKa of Acetic acid and verification of Ostwald dilution law. 6. Potentiometry/pH metry a. Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter. b. Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH. c. Determination of the dissociation constant of monobasic/dibasic acid by Albert-Serjeant method. d. Determination of Redox potential of Fe++/Fe+++ system. 7. Polarimetry a. Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter. b. Enzyme kinetics –inversion of sucrose. c. Determine the specific and molecular rotation of optically active substances. 8. Error analysis and statistical data analysis a. Linear Regression Analysis b. Curve Fitting c. Student "t" Test d. Data Analysis Using Basic Statistical Parameters e. Calibration of volumetric Apparatus, Burette, Pipette Weight Box etc. 9. Use of computer programmes The students will learn how to operate a PC and how to run standard programmes and packages. Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmes. Monte Carlo and Molecular dynamics. Programmes with data preferably from physical chemistry laboratory. Further, the student will operate one or two or the packages such as Microsoft excel, word, power point, SPSS, Origin, Matlab and Easyplot.
Course Outcome	• On the completion of this course successfully student will be gain the practical knowledge for performing the experiments of spectroscopy and

	physical and analytical chemistry laboratory work.
Text Books	1. Experiments and Techniques in Organic Chemistry, D.Pasto, C. Johnson and M.Miller, Prentice Hall. 2. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Heath. 3. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold. Handbook of Organic Analysis –Qualitative and Quantitative, H. Clark, Adward Arnold. 4. Vogel's Textbook of Practical Organic Chemistry, 5. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman. 6. Findley's Practical Physical Chemistry, B.P. Levi
Reference Books	1. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill. 2. Computer and Common Sense, R. Hunt and J. Shelley, Prentice Hall. 3. Computational Chemistry, A.C. Norris. 4. Microcomputer Quantum Mechanics, J.P. Killngbeck, Adam Hilger. 5. Computer Programming in FORTRAN IV, V. Rajaraman, Prentice Hall. 6. An Introduction to Digital Computer Design, V. Rajaraman and T. Radhakrishnan, Prentice Hall.Experiments in Chemistry, D.V. Jahagirgar.

Two year Master of Science in Chemistry programme
M.Sc. Chemistry Semester-I
2022-2023

<table>
<tr><td>Course Title</td><td colspan="5">COMPUTER APPLICATION AND CHEMOINFORMATICS</td></tr>
<tr><td>Course Code</td><td colspan="5">SMS04121T</td></tr>
<tr><td rowspan="2">Course Credit</td><td>L</td><td>T</td><td>P</td><td>TC</td><td></td></tr>
<tr><td>2</td><td>-</td><td>-</td><td>2</td><td></td></tr>
<tr><td>Prerequisite</td><td colspan="5">Students must have the basic knowledge of computer and chemistry</td></tr>
<tr><td>Objective</td><td colspan="5">• Computers for Chemists in advance and establish foundation to research in the respective domain.</td></tr>
<tr><td>Course Content</td><td colspan="5">UNIT-I
Computer Basics, Introduction to computer networks, LAN, MAN, WAN & Internet, Internet applications. Introduction to MS office, working with documents, worksheets and presentations
UNIT-II
Concepts of Programming languages, Introduction to ‘C’ language, flowcharts and algorithms, introduction to data structure and database concepts, Object oriented concepts.
UNIT-III
Introduction to Chemoinformatics: History and evolution of chemoinformatics, Use of chemoinformatics, Prospects of chemoinformatics, Molecular Modelling and Structure elucidation.
UNIT-IV
Representation of molecules and chemical reactions: Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification, Searching chemical structures: Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.
UNIT-V
Applications: Prediction of Properties of Compounds; Linear Free Energy Relations; Quantitative Structure-Property Relations; Descriptor Analysis; Model Building; Modeling Toxicity; Structure-Spectra correlations; Prediction of NMR, IR and Mass spectra; Computer Assisted Structure elucidations; Computer Assisted Synthesis Design, Introduction to drug design; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Virtual Screening; Design of Combinatorial Libraries; Ligand-Based and Structure Based Drug design; Application of Chemoinformatics in Drug Design.</td></tr>
</table>

Course Outcome	• On the completion of this course successfully student will be able to understand the development of mathematics,biology and computers for chemists
Text Books	1. Let us learn C : Yashwant Kanetkar 2. Mastering C: Venugopal 3. Gasteiger, J. & Engel,T. (2003) Chemoinformatics: Atext-book.Wiley-VCH.
Reference Books	1. Andrew R. Leach &Valerie, J.Gille t(2007) An introduction to Chemoinformatics. Springer: The Netherlands. 2. Gupta,S.P.(2011)QSAR&MolecularModeling.AnamayaPub.:NewDelhi.