Semester Syllabus for M. Sc. in Chemistry w.e.f. 2023-25 Academic Year

FIRST SEMESTER			
Course No	**Course Title**	**Credit**	**Mark**
CH-411	INORGANIC CHEMISTRY-I	04	100
CH -412	ORGANIC CHEMISTRY-I	04	100
CH -413	PHYSICAL CHEMISTRY-I	04	100
CH -414	INSTRUMENTAL METHODS OF ANALYSIS	04	100
CH -415	INORGANIC PRACTICAL-I	02	50
CH -416	ORGANIC PRACTICAL-I	02	50
	Total	**20**	**500**
In addition to this student(s) has to take either Environmental Studies or Disaster Management of 2 credit. The detail course will be available in the University website.			
SECOND SEMESTER			
Course No	**Course Title**	**Credit**	**Mark**
CH -421	INORGANIC CHEMISTRY-II	04	100
CH -422	ORGANIC CHEMISTRY-II	04	100
CH -423	PHYSICAL CHEMISTRY-II	04	100
CH -424	ATOMIC &MOLECULAR SPECTROSCOPY	04	100
CH -425	INORGANIC PRACTICAL-II	02	50
CH -426	ORGANIC PRACTICAL-II	02	50
	Total	**20**	**500**

1. ***In addition to this student(s) has to take one Inter Departmental Course of 3 credit offered by other departments. The detail course will be available in the University website.***
2. ***Also, the student has to opt for one MOOCS course of 03 credit through Swayam, NPTEL etc platform.***

THIRD SEMESTER			
Course No	**Course Title**	**Credit**	**Mark**
CH -511	INORGANIC CHEMISTRY-III	04	100
CH -512	ORGANIC CHEMISTRY-III	04	100
CH -513	PHYSICAL CHEMISTRY-III	04	100
CH -514	ANALYTICAL TECHNIQUES IN ORGANIC CHEMISTRY	04	100
CH -515	PHYSICAL CHEMISTRY PRACTICAL	02	50
CH -516	COMPUTATIONAL CHEMISTRY PRACTICAL	02	50
	Total	**20**	**500**
In addition to this student(s) has to takeEntrepreneurship Development Program Course of 2 credit. The detail course will be available in the University website.			
FOURTH SEMESTER			
Course No	**Course Title**	**Credit**	**Mark**
CH -521	ADVANCED ORGANOMETALLIC CHEMISTRY	04	100
CH -522	ADVANCED ORGANIC SYNTHESIS OR ADVACED ANALYTICAL CHEMISTRY OR PHOTOPHYSICAL CHEMISTRY	04	100
CH -523	SUPRAMOLECULAR CHEMISTRY OR CHEMISTRY OF NANOMATERIALS OR COMPUTATIONAL CHEMISTRY	04	100
CH -524	PROJECT	04	100
CH -525	COMPREHENSIVE VIVA	02	50
CH -526	SEMINAR	02	50
	Total	**20**	**500**

In addition to this the student has to take YuvaSanskar and to give preference for either NCC or NSS course.

FIRST SEMESTER

CH-411	**INORGANIC CHEMISTRY-I**	**4 credits**
UNIT-I:	**Basic Concepts of Symmetry and Group Theory**	
	Symmetry operation, symmetry element, classification of symmetry elements, definition of group, subgroup, cyclic groups, molecular point groups, group multiplication table, group generators, symmetry of platonic solids, conjugacy relation and classes, matrix representation of symmetry elements, character of a representation, reducible and irreducible representation, properties of irreducible representation.	
UNIT-II:	**Group Theory and Spectroscopy**	
	Character table (explanation and significance), construction of character tables for C_{2v}, C_{3v}, $C_{4v,}$ $C_{2h,}$ D_{2d} and D_4 point groups, direct product, standard reduction formula, applications of group theoretical methods for selection rules in: infrared spectroscopy, Raman spectroscopy and electronic spectroscopy.	
UNIT-III:	**Theories of Metal-Ligand Bonding**	
	Basic concepts of crystal field theory (CFT), molecular orbital theory (MOT): classification of metal valence orbitals into sigma symmetry, ligand group orbitals (LGOs) of sigma symmetry, LGOs of pi symmetry, molecular orbital energy level diagrams for octahedral and tetrahedral complexes, concept of ligand field theory (LFT).	
UNIT-IV:	**Term Diagram, Electronic Spectral and Magnetic Properties of Metal Complexes**	
	Concept of term symbols, derivation of term symbol for pn and dn configurations, Orgel diagram for dn configurations, Significance of Tanabe-Sugano diagram. Electronic spectra of metal complexes, selection rules, relaxation in selection rules, evaluation of Dq, B and beta(β) parameters for the complex with T1 ground state and A2 ground state, spectrochemical series and nephlelauxetic series, charge transfer spectra. Concept of magnetic properties of metal complexes.	
TEXT BOOKS:	1. *Chemical Applications of Group Theory by F. A. Cotton, Wiley India (P) Ltd., 3rd edn, 2009, New Delhi.* 2. *Symmetry and Spectroscopy of Molecules by K. V. Ready, New Age International Ltd. 2nd edn, 2009, New Delhi.* 3. *Symmetry and Group Theory in Chemistry by R. Ameta, New Age International Ltd., 1st edn, 2013, New Delhi.* 4. *Solid State Chemistry by D. K. Chakravarty, New Age International Limited, 1996, New Delhi.* 5. *Advanced Inorganic Chemistry by F. A. Cotton and G. Wilkinson, Wiley India (P) Ltd., New Delhi, 6th edition, 1999.* 6. *Fundamental concepts of Inorganic Chemistry (vol-5, and vol-6) by Asim K. Das and Mahua Das, CBS publishers and distributors, 2nd Edition,2019.*	
REFERENCE BOOK	1. *Inorganic Chemistry by G. L. Miessler and D. A. Tarr, Pearson Education, 3rd edn, 2004.* 2. *Inorganic Chemistry (Principles of Structure and Reactivity) by James E. Huheey, Ellen A. Keiter,Richard L. Keiter and Okhil K.Medhi Pearson Education, 4th edn, 2006.*	
CH-412	**ORGANIC CHEMISTRY I**	**4 credits**
UNIT-I:	**Aromaticity and Electronic Effects**	
	Delocalized chemical bonding, Conjugation, Cross conjugation, Electronic effect, Aromaticity in benzenoid and non-benzenoid compounds, Huckel's rule, Alternant and non-alternant hydrocarbons, Energy levels in odd and even-alternant hydrocarbons, energy levels of π-molecular orbitals, Aromaticity of annulenes and heteroannulenes, Anti-aromaticity, Homo-aromaticity. Classification of reactions and mechanisms, Kinetic and thermodynamic control reactions, Hammond's postulate, Transition states and intermediates in Potential energy diagrams,The Hammett equation and linear free energy relationship, Substituent and reaction constants, Hard and soft acids and bases. Effect of structure on the strengths of acids and bases.	
UNIT-II:	**Aliphatic Substitution Reactions**	
	Nuceleophilic substitution – S_N2, $S_N1$and SET mechanisms. Neighboring group participation by σ and π-bonds, anchimeric assistance. Carbocation rearrangements, Nucleophilic substitution at an aliphatic trigonal, allylic and a vinylic carbon.	

	Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity. Electrophilic substitution reactions – S_E1, S_E2 and S_Ei mechanisms, Effect of substrate, leaving group and solvent, Reactions (hydrogen exchange, migration of double bonds, keto-enol tautomerism, halogenation, aliphatic diazonium coupling, Stork-enamine reaction).
UNIT-III:	**Aromatic Substitution Reactions**
	Aromatic electrophilic substitution reactions – The arenium ion mechanism. Orientation and reactivity. Energy profile diagrams. Structure reactivity relationship in mono-substituted benzene, Quantitative treatment of reactivity in substrates and electrophiles. orientation in benzene and higher order rings with one or more than one substituent, Diazonium coupling, Vilsmeir - Haack reaction, Gatterman reaction, Gatterman-Koch reaction, Hoesch reaction Pechmann reaction. Aromatic Nucleophilic Substitution – ArS_N1, ArS_N2, benzyne, Effect of substrates, leaving groups, and attacking nucleophile, Reactions: Nucleophilic displacement in areno-diazonium salts by different nucleophiles, Goldberg reaction,Schiemann reaction,Chichibabin reaction. Free radical Substitution: Intermediates, Reaction at sp^2 carbon, Reactivity in aliphatic, at bridge head position and in aromatic substrates.
UNIT-IV:	**General Stereochemistry**
	Chirality, Fischer projection and R and S notations, Threo and erythro nomenclature, E and Z nomenclature, Optical isomerism in biphenyls and allenes, Concept of Prostereoisomerism and Asymmetric synthesis, Conformation of a few acyclic molecules (alkanes, haloalkanes), Conformation of cyclic systems having one and two sp2 carbon atoms.
TEXT BOOKS:	1. *Organic Chemistry (Second Edition), by J. Clayden, N. Greeves, S. Warren.* 2. *Organic Reactions and Their Mechanisms by P S Kalsi, New Age International Private Limited; Fifth edition, 2020* 3. *Organic Reaction Mechanisms by Raj K. Bansal, New Age International Private Limited, 2012* 4. *Mechanism and Theory in Organic Chemistry by Lowry and Richardson (Harper Row Publishers, New York)* 5. *A Guidebook to Mechanism in Organic Chemistry by Peter Sykes* 6. *Jonathan Clayden, Nick Greeves, and Stuart Warren. "Organic Chemistry," Oxford University Press, 2014.* 7. *D. Nasipuri, Stereochemistry of Organic Compounds Principles and Applications, New Age International Publishers, 3rd Edition, 2011* 8. *Stereochemistry: Conformation and Mechanism by P.S. Kalsi New Age Publishers; Tenth Edition, 2019*
REFERENCE BOOKS:	1. *Advanced Organic Chemistry: Reaction Mechanism and Structure by Jerry March (Wiley Eastern Limited)* 2. *W. Carruthares, Iain coldham, Modern Methods of Organic Synthesis South Asia Edition, Cambridge University Press, Fourth Edition, 2015.* 3. *F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry Part B: Reaction and Synthesis, Springer, 5th Edition, 2010.* 4. *Stereochemistry of Organic Compounds by Ernest L. Eliel Wiley; 1st Edition, 2008*
CH-413	**PHYSICAL CHEMISTRY I** **4 credits**
UNIT-I	***Chemical Kinetics & Fast Reaction***
	Theories of reaction rates, Collision theory, Transition state theory, Arrhenius equation and the activated complex theory, Reaction between ions, Salt effect, Steady-State Kinetics, Kinetic and Thermodynamic concept of Reactions, Treatment of unimolecular reaction (Lindeman-Hinshelwood and Rice-Ramspeger-Kassel-Marcus (RRKM) theories), Dynamic chain (H_2 + Br_2 reaction, pyrolysis of CH_3CHO, Decomposition of ethane). Study of Fast reactions by relaxation, Stopped flow and Flash photolysis methods.
UNIT-II	***Polymer Chemistry***
	Polymer-definition, Classification of polymer, Polymer structure, Number average and molecular weight average, Step growth & chain growth polymerization, Kinetics of polymerization, Stereochemistry of polymerization.
UNIT-III	***Adsorption & Catalysis***

	Adsorption, types of adsorption, Gibbs adsorption isotherm, Freundlich's adsorption isotherm, Langmuir's adsorption isotherm and its limitations, BET adsorption isotherm and its applications, Heat of adsorption, estimation of surface areas of solids from solution adsorption studies, Enzyme Catalysis & Heterogeneous Catalysis.	
Unit-IV	***Phase Rule***	
	Concept of Equilibrium between phases, Derivation of phase rule, Ideal Solution, Liver Rule, Brief concept on one and two component system, Application of phase rule to three component systems of both solids and liquids.	
TEXT BOOKS:	1. *Chemical Kinetics by K.J. Laidler, Pearson; 3rd edition (1997)* 2. *Textbook of Physical Chemistry by K L Kapoor, McGraw Hill (2014)* 3. *Principles of Physical Chemistry by B.R. Puri, L.R. Sharma, M.S. Pathania, Vishal Publishing Co, 47th Edition (2016)* 4. *Polymer Science by Gowariker, Viswanathan & Sreedhar*	
REFERENCE BOOKS:	1. *Advanced Physical Chemistry by D.N. Bajpai, S. Chand; 2nd edition (1992)* 2. *Atkins' Physical Chemistry by P. W. Atkins and Julio de Paula, , Oxford; 10th Edition (2014)* 3. *Reaction Kinetics by Pilling &Seakins* 4. *Physical Chemistry Through Problems by Dogra & Dogra*	
CH -414	**INSTRUMENTAL METHODS OF ANALYSIS**	**4 credits**
UNIT-I	**Atomic Absorption and Flame Emission Spectroscopy**	
	Basic Principle of atomic absorption spectroscopy (AAS), instrumentation, atomization techniques, application of AAS, sensitivity of instruments, strengths and limitations of atomic absorption spectroscopy. Basic principle of flame emission spectroscopy (FES), instrumentation, application of FES, limitations in FES.	
UNIT-II	**Electroanalytical Method**	
	Polarography: principle, instrumentation, Ilkovic equation, Significance of half wave potential, application of polarography. Cyclic voltammetry: principle, instrumentation, and its application, ion selective electrodes.	
UNIT-III	**Thermoanalytical Methods**	
	Thermogravimetric analysis (TGA): Principle, instrumentation, factors affecting TGA curve, derivative thermogravimetric analysis (DTGA) and application of thermogravimetric analysis, differential thermal Analysis (DTA), instrumentation of DTA and application of DTA, simultaneous study of TGA, DTA with examples. differential scanning calorimetry (DSC) and thermometric titration.	
UNIT-IV	**Chromatography**	
	Principle and applications of thin layer chromatography (TLC), column chromatography (LC), gas chromatography (GC), high pressure column chromatography (HPLC).	
TEXT BOOKS:	1. *Analytical Chemistry (Theory and Practice) by U.N. Dash, Sultan Chand & Sons Pvt. Ltd., New Delhi, 2013.* 2. *Basic concept of Analytical Chemistry by S. M. Khopkar, New Age International (P) Ltd. Publishers, 3rd Edition, 2008.* 3. *Instrumental Methods of Chemical Analysis by Gurdeep R. Chatwal, Sham K. Anand, Himalaya Publishing House, 5th Edition,2014.*	
REFERENCE BOOKS	1. *Quantitative Analysis by Vogel, Pearson Education Ltd., New Delhi, 6th edition, 2009.* 2. *Instrumental Method of Analysis by H. Willard, L. Merritt, J. Dean & F. Settle, CBS publisher and distributors Pvt. Ltd., 7th edition, 2004.*	
CH -415	**INORGANIC CHEMISTRY PRACTICAL-I**	**2 credits**
	Analysis of an inorganic mixture containing not more than 6 radicals. The mixture will include rare earth like Tungstate, Vanadate, Molybdate and Cerium (IV). Insoluble matters and other interfering radicals will also be included. Organic radicals are excluded.	
BOOKS:	1. *Vogel's Qualitative Inorganic Analysis, 7th edition; Revised by G. Svehla.* 2. *Vogel's Text Book of Quantitative Chemical Analysis, 5th Revised by G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny.* *Advanced Practical Inorganic Chemistry, 22nd edition; By Gurdeep Raj*	
CH -416	**ORGANIC CHEMISTRY PRACTICAL-I**	**2 credits**
	Isolation and identification of multi-functional compounds in a mixture of two organic compounds.	
BOOK:	*Advanced Practical Organic Chemistry, 3/e by N K Vishnoi*	

SECOND SEMESTER

CH -421	**INORGANIC CHEMISTRY-II**	**4 credits**
UNIT-I	**Complexes of Carbon Monoxide and its Analogs**	
	Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important synthesis and reactions of metal carbonyls, carbonylate anions and carbonylate hydride, carbonyl halides; preparation, bonding and important reactions of transition metal complexes with isocyanide, cyanide, dinitrogen, carbon disulphide and nitrogen monoxides; chemistry of carbenes and carbynes.	
UNIT-II	**Metal Cluster and Polyacids**	
	Concept of metal cluster, bonding in metal clusters, metal carbonyl type clusters, anionic and hydride clusters, method of synthesis, super large cluster, electron counting in medium size cluster (Wade's rule, capping rule), isolobal relationship, clusters of Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, Pt metals and their synthesis and reactions, Catalysis by metal cluster. Polyacids**:** definition, classification, polymerization of chromate, isopoly acids and anions, synthesis of isopoly acids, structures of isopolymolybdates, isopolytungstates and isopolyvanadates, heteropoly acids of W and Mo. Applications of isopoly and heteropoly compounds.	
UNIT-III	**Biomolecular Storage and Transportation of ions**	
	Lipids, lipid bilayer, biological membranes, Ramachandran's plot, biologically important metal ions (Na, K, Mg, Ca, Cu, Fe, Zn, Co and Mo) and their functions, passive and active transport processes, Na^+/K^+ pump, calcium pump, ionophores, storage and transport of iron, copper and zinc, siderophores, ferritin and transferrin in regard to iron-storage and transportation. Chemistry of porphyrin, iron porphyrins (heme proteins): hemoglobin (Hb), myoglobin (Mb) and their behavior as oxygen carrier, O_2 affinity, cooperativity and Bohr's effect, heme protein as electron carrier with particular reference to cytochrome-c and cytochrome-450, and cytochrome oxidase. Catalases and peroxidases. non-heme oxygen uptake protein (hemerythrin and hemocyanin). Magnesium porphyrins (Chlorophyll): Photosynthesis, the light and dark reaction (Calvin cycle). Non-heme iron-sulphur protein as electron carrier, rubredoxins and ferredoxins.	
UNIT-IV	**Biomolecular Catalysis**	
	Basic concepts of amino acids, peptides and proteins, structures of proteins, preliminary idea about enzyme, cofactor, co-enzyme, apoenzyme, prosthetic group, metal-activated enzyme and metalloenzyme. biological significance and mechanistic aspects of carboxypeptidase, carbonic anhydrase, blue-oxidases, non-blue oxidases, superoxide dismutase, structure and biological functions of molybdenum nitrogenase.	
TEXT BOOKS:	1. *Advance Inorganic Chemistry by F.A. Cotton, G. Wilkinson & C. Murillo, Wiley Publication, 6th edition, 1999.* 2. *Inorganic Chemistry (Principles of Structure and Reactivity) by James E. Huheey, Ellen A. Keiter, Richard L. Keiter and Okhil K. Medhi, Pearson Education, 4th edn, 2006.* 3. *Modern Aspect of Inorganic Chemistry by Emelius and Sharpe, Routledge & Kegan Paul PLC, England, 4th revised edition, 1978.* 4. *Bio-Inorganic Chemistry by Asim K Das.* 5. *Bio-Inorganic Chemistry by E. Ochia.* 6. *Bioorganic, BioInorganic and Supramolecular Chemistry by P. S. Kalsi and J. P. Kalsi.* 7. *Inorganic Chemistry (4thEdn) by Huheey, Keiter, Keiter and Medhi.* 8. *Bioinorganic and Suparmolecular Chemistry by A. Bhagi and G. R. Chatwal..*	
REFERENCE BOOKS	1. *Inorganic Chemistry by G. L. Miessler and D. A. Tarr, Pearson Education, 3rd edn, 2008.* 2. *Comprehensive Coordination Chemistry, by Wilkinson, Gillarsand, Pergamon Press, 1989.*	
CH-422	**ORGANIC CHEMISTRY II**	**4 credits**
UNIT-I	**Addition Reactions**	

	Addition to C=C multiple bonds – Electrophilic, Nucleophilic and Free radical. Reactions: Hydroboration, Michael reaction, Sharpless Asymmetric epoxidation. Addition to carbon-heteroatom multiple bonds: Mechanism and reactivity, Reactions: $LiAlH_4$ reduction of carbonyl compounds, acids, esters, nitriles, addition of Grignard reagents to carbonyl compounds, Reformatsky reaction, Aldol condensation, Knoevenagel condensation, Perkin reaction, Mannich reaction, Wittig reaction, Stobbe reactions, Tollens reaction, Benzoin condensation.
UNIT-II	**Elimination Reactions**
	E_1, E_2, E_1CB and E_2CB mechanisms, Orientation, Effect of substrate, base, leaving group and medium, Orientation of double bond, Sayetzeff and Hoffman rules, Pyrolytic elimination reaction, Oxidative elimination (oxidaton of alcohol by chromium, Moffatt oxidation). Reactions: Cleavage of quaternary ammonium hydroxides, Chugaev reaction, Shapiro reaction.
UNIT-III	**Mechanistic Considerations**
	Nature of migration, migratory aptitude, memory effects. Rearrangements: Wagner-Meerwein, Favorskii, Fries, Carbene intermediate, Arndt-Eistert synthesis, Neber, Nitrene intermediates (Beckmann, Hofmann, Schmidt, Lossen, Curtius), Baeyer-Villiger, Shapiro reaction, Von-Richter, Sommelet-Hauser rearrangement.
UNIT-IV	**Dynamic Stereochemistry**
	Conformation and reactivity, Selection of substrates, Quantitative correlation between conformation and reactivity, (Weinstein-Eliel equations and Curtin-Hammett principles), Conformational effects on stability and reactivity in acyclic compounds (ionic elimination, intramolecular rearrangements) and in cyclic systems, (Nucleophilic substitution reaction at ring carbon, Formation and Cleavage of epoxide rings, Addition reactions to double bonds, Elimination reactions). Stereospecific and stereoselective reactions.
TEXT BOOKS:	*1. Organic Chemistry (Second Edition), by J. Clayden, N. Greeves, S. Warren.* *2. Organic Reactions and Their Mechanisms by P S Kalsi, New Age International Private Limited; Fifth edition, 2020* *3. Organic Reaction Mechanisms by Raj K. Bansal, New Age International Private Limited, 2012* *4. Mechanism and Theory in Organic Chemistry by Lowry and Richardson (Harper Row Publishers, New York)* *5. A Guidebook to Mechanism in Organic Chemistry by Peter Sykes* *6. Jonathan Clayden, Nick Greeves, and Stuart Warren. "Organic Chemistry," Oxford University Press, 2014.* *7. D. Nasipuri, Stereochemistry of Organic Compounds Principles and Applications, New Age International Publishers, 3rd Edition, 2011* *8. Stereochemistry: Conformation and Mechanism by P.S. Kalsi New Age Publishers; Tenth Edition, 2019*
REFERENCE BOOKS:	*1. Advanced Organic Chemistry: Reaction Mechanism and Structure by Jerry March (Wiley Eastern Limited)* *2. W. Carruthares, Iain coldham, Modern Methods of Organic Synthesis South Asia Edition, Cambridge University Press, Fourth Edition, 2015.* *3. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry Part B: Reaction and Synthesis, Springer, 5th Edition, 2010.* *4. Stereochemistry of Organic Compounds by Ernest L. Eliel Wiley; 1st Edition, 2008*
CH-423	**PHYSICAL CHEMISTRY II** **4 credits**
UNIT-I	***Classical Thermodynamics***
	Brief resume of the concepts of laws of thermodynamics, Free energy, chemical potential and entropy, Third law of thermodynamics and determination of entropy, Entropy and probability, Boltzmann-Planck equation, Partial molar properties (partial free energy, molar volume and molar heat content), Their significance and determination. Concept of fugacity and its determination.
UNIT-II	***Classical and Quantum Statistical Mechanics***
	Concept of probability, Starling approximations, Most probable distribution,

	System, Phase Space, μ-Space, ϒ-Space, Liouville's Theorem, Statistical Equilibrium, Brief Concepts on Ensembles, Canonical, Grand Canonical and Micro-canonical ensembles. Bose-Einstein statistics, Fermi-Dirac statistics and Maxwell-Boltzmann statistics
UNIT-III	***Partition Functions & Statistical Thermodynamic Properties of Solids***
	Significance of partition function, Calculation of thermodynamic properties and equilibrium constant in terms of partition functions, Evaluation of transnational, vibrational and rotational partition function for monoatomic and polyatomic ideal gases, electronic partition function. Some thermal characteristics of crystalline solids, Classical treatment of solids, Einstein Model, Debye Modification, Limitation and modification of Debye theory.
UNIT-IV	**Computer Application in Chemistry**
	Basic structure of a computer: The CPU, the I/O devices, the internal memory, commonly used secondary storage media. Data representation: Overview of binary, octal and hexadecimal number system. The software: Concept of low level and high-level languages, Compiler interpreter, editor, operating system concepts, salient features of Windows and LINUX operating systems. Algorithm, Flowchart, Decision-table, elements of high-level programming languages. Application of numerical methods to chemical problems.
TEXT BOOKS:	*1. Text Book of Physical Chemistry by K.L. Kapoor* *2. Principles of Physical Chemistry by Puri, Sharma &Pathania* *3. Chemical Thermodynamics by Rastogi & Mishra* *4. Thermodynamics for Chemists by S. Glasstone* *5. Molecular Thermodynamics by McQuarrir& Simon* 6. *Statistical Thermodynamics by M. C. Gupta* 7. *Computational Chemistry by A.C. Norris*
REFERENCE BOOKS:	*1. Advanced Physical Chemistry by D.N. Bajpai, S. Chand; 2nd edition (1992)* 2. *Atkins' Physical Chemistry by P. W. Atkins and Julio de Paula, , Oxford; 10th Edition (2014)* 3. *Physical Chemistry Through Problems by Dogra & Dogra* 4.
CH-424	**ATOMIC &MOLECULAR SPECTROSCOPY** | **4credits**
UNIT-I	***Atomic Spectroscopy***
	The electromagnetic spectrum, A general discussion on various molecular excitation processes, Spectra of hydrogen and hydrogen like atoms, alkali metals spectra, L-S coupling, Term symbols, Space quantisation, Zeeman effect, Stark effect, Paschen-Back effect.
UNIT-II	***Vibrational & Rotational Spectroscopy & Raman Spectroscopy***
	Molecular Spectra of Diatomic Gases, Classification of molecules, Rotational Spectra, Vibrational Spectra, Vibrational-Rotational Spectra, P, Q and R Branches. Theory of Raman spectra, Rotational Raman spectra, Vibrational Raman spectra, Rotational-Vibrational Raman spectra, comparison with IR spectra.
UNIT-III	***Electron Spin Resonance Spectroscopy***
	Theory, instrumentation, g-values, hyperfine splitting, ESR spectra of systems with more than one unpaired electron, double resonance, ENDOR and ELDOR techniques.
UNIT-IV	***Photoelectron &Mossbauer Spectroscopy***
	Principles of Photoelectron spectroscopy, ultraviolet photoelectron spectra and their interpretation Principles of Mossbauer spectroscopy, Experimental methods, Theoretical aspects, Quadrupole splitting, Magnetic hyperfine interaction.
TEXT BOOKS:	*1. Fundamentals of Molecular Spectroscopy by C.N. Banwell* *2. Fundamentals of Molecular Spectroscopy by G.M. Barrow* *3. Molecular Spectroscopy, P.S. Sindhu*
REFERENCE BOOKS:	*1. Advanced Physical Chemistry by D.N. Bajpai, S. Chand; 2nd edition (1992)* *2. Atkins' Physical Chemistry by P. W. Atkins and Julio de Paula, , Oxford; 10th Edition (2014)* *3. Physical Chemistry Through Problems by Dogra & Dogra* *4. Spectroscopy Vol. I & II by Walker & Straw*

CH-425C	**INORGANIC CHEMISTRY PRACTICAL-II**	**2 credits**
	1. Principle of estimation of the main constituents of Brass and Portland Cement. (a) Estimation of Ca and Mg in a given solution prepared from a sample of cement by EDTA method. (b) Estimation of Cu in a given solution prepared from a sample of Brass. 2. Preparation and characterization of the following inorganic compounds: (i) Tetramminecupricsulphate $[Cu(NH_3)_4]SO_4 .H_2O$ (ii) Sodium cobaltinitrite , $Na_3[Co(NO_2)_6]$ (iii) Potassium chromioxalate , $K_3[Cr(C_2O_4)_3]$.	
BOOK:	*1. Vogel's Qualitative Inorganic Analysis, 7th edition; Revised by G. Svehla.* *2. Vogel's Text Book of Quantitative Chemical Analysis, 5th Revised by G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny.* *3. Advanced Practical Inorganic Chemistry, 22nd edition; By Gurdeep Raj*	
CH-426	**ORGANIC CHEMISTRY PRACTICAL-II**	**2 credits**
	1. Preparation of benzoin, benzil and benzillic acid from benzaldehyde. 2. Preparation from p-idotoluene from p-toluidene. 3. Preparation of ethyl acetoacetate from ethyl acetate. 4. Estimation of nitrogen by Kjeldahl method. 5. Estimation of keto group by gravimetric method. 6. Dibenzalacetone from benzaldehyde. 7. Cannizaro reaction – 4-chloro benzaldehyde as substrate. 8. Grignard reaction – synthesis of triphenyl methanol from benzoic acid.	
BOOK:	*Advanced Practical Organic Chemistry, 3/e by N K Vishnoi*	

THIRD SEMESTER

CH -511	**INORGANIC CHEMISTRY-III**	**4 credits**
UNIT-I	**Substitution Reactions in Octahedral Complexes**	
	Nature of substitution reactions, kinetic application of Crystal Field Theory, acid hydrolysis of octahedral Co(III) complexes with reference to effect of charge, chelation, steric crowding & effects of leaving group, base hydrolysis of octahedral Co(III) complexes: Conjugate base mechanism, test of conjugate base mechanism, anation reaction, substitution reaction without cleavage of metal-ligand bond.	
UNIT-II	**Substitution Reactions in Square Planar Complex and Redox Reactions**	
	Thermodynamic and kinetic stability, trans effect and its synthetic applications, theories of trans effect (polarization &π -bonding theories), factors affecting the rate law and reaction profile (leaving group, steric group, charge, electrophillic catalysis, nucleophile and temperature). Redox reactions: electron tunneling hypothesis, concept of Marcus-Hush theory, atom transfer reactions, one and two electron transfer, complementary and non-complementary reactions, inner sphere and outer sphere reactions, electron transfer through extended bridges, concept of hydrated electron.	
UNIT-III	**Nuclear Chemistry**	
	Nuclear stability, magic numbers, radioactivity, general characteristics of radioactive decay particles, decay kinetics, nuclear reaction, Bethe's notation, types of nuclear reaction, nuclear cross section, compound nuclear theory, nuclear fission, liquid drop model, shell model, hard core preformation theory, fission fragments and their mass distribution, charge distribution, ionic charge of fission fragments, working principle of nuclear reactor, concept of nuclear fusion, concept of boron-neutron capture therapy.	
UNIT-IV	**Solid State Chemistry**	
	General idea of crystal lattice, unit cell, classification of crystals, crystal planes, Miller indices, Bragg's law and applications, determination of cubic crystal structure from systematic absences in diffraction pattern, perfect and imperfect crystals, point defects, stoichiometry defects, Schottky defects and Frenkel defects, thermodynamics of Schottky and Frenkel defects, bonding in ionic solids, colour centers, non-stoichiometry defects, band structure of solids.	
TEXT BOOKS:	*1. Mechanisms of Inorganic Reactions byF. Basolo and R. G. Pearson.* *2. Inorganic Chemistry by Asim K Das.* *3. Inorganic Chemistry by Cotton and Wilkinson (4thEdn).* *4. Essentials of Nuclear Chemistry by H. J. Arniker* *5. Solid State Chemistry by D. K. Chakravarty, New Age International Limited, 1996, New Delhi.*	
REFERENCE BOOKS	*1. Solid State Chemistry and its Applications by A.R. West, Wiley, 1989, 2nd edition, Singapore.* *2. Principles of the Solid State by H.V. Keer, Wiley Eastern. Limited, 1993, New Delhi.*	
CH-512	**ORGANIC CHEMISTRY III**	**4 credits**
UNIT-I	**Organic Redox Reaction**	
	Oxidation: Oxidation of hydrocarbons, oxidation of alcohols by various reagents, oxidation of carbon-carbon double bonds to diols and epoxides, Chromium (VI), Manganese (VII) oxidants, Oxidation with peracids, with hydrogen peroxide, with singlet oxygen. with iodobenzene diacetate, and thallium (III) nitrate. Reduction: Catalytic hydrogenation, selectivity of reduction, Reduction by hydride transfer reagents: Aluminiumalkoxid, Sodium borohydride ($NaBH_4$), di-isobutylaluminium hydride, Sodium cyanoborodydride, Lithium trialkylborohydride, reduction with hydrazine, reduction with trialkyltinhydride, the Birch reduction, the Wolff-Kischner reduction, the Cannizarro reduction, the Resenmund reduction.	
UNIT-II	**Pericyclic Reaction and Photochemistry**	
	Pericyclic reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann rules, Correlation diagrams and FMO approach. Electrocyclic reactions - Conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems.	

	Cycloaddition reactions - suprafacial and antarafacial additions, 4n and 4n+2 systems, thermal and photochemical processes, 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements - [i,j] shifts of C-H and C-C bonds;Sommelet-Hauser,Claisen, thio-Claisen, Cope and aza-Cope rearrangements. Ene reaction. Photochemical processes:Fluorescence, Phosphorescence, excimers and exciplex formation, Photochemical reactions: Cis-Trans Isomerization, photochemical dissociation, Reduction of ketones, Paterno-Buchi reaction, Norrish type I and II reactions, Di-π-methane rearrangement, Photochemistry of arenes, Barton reaction.
UNIT-III	**Reagents in Organic Synthesis**
	Gilman's reagent, Lithium dimethyl cuprate, Lithium diisopropyl amide, DCC, 1,3-Dithiane, Trimethyl silyl iodide, Tri-n-butyl tin hydride, Osmium tetroxide, Selenium dioxide, Phase transfer catalysis (Crown ether, Merrifield resin, Wilkinson's catalyst), Dichlorodicyano benzoquinone (DDQ).
UNIT-IV	**Retrosynthetic Approach**
	Synthetic design: Introduction, Retrosynthetic approach, Terminology in Retro synthetic analysis, One group disconnection, (alcohol, carbonyl compound, olefins and acids), Two group disconnections (β-hydroxy compounds,α, β-unsubstituted carbonyl compounds, 1,3-dicarbonyl compounds, 1,5 dicarbonyl compounds), Synthesis of some organic molecules by disconnection approach.
TEXT BOOKS:	1. *Reactions, Rearrangements and Reagents by S.N. Sanyal, Bharati Bhawan Publishers & Distributors; Fourth edition, 2019* 2. *Organic Reaction Mechanisms by Raj K. Bansal, New Age International Private Limited, 2012* 3. *Synthetic Approaches in Organic Chemistry, R.K. Bansal, Narosa Publishing House,India, 1996* 4. *Jonathan Clayden, Nick Greeves, and Stuart Warren. "Organic Chemistry," Oxford University Press, 2014.* 5. *Organic Reactions and Orbital Symmetry by Gilchrist and Storr, Cambridge University Press; 2nd Edition 1979* 6. *Mechanism and Theory in Organic Chemistry by Lowry and Richardson (Harper Row Publishers, New York)* 7. *Photochemistry and Pericyclic Reactions by Jagdamba Singh and Jaya Singh, NEW AGE; 3rd Edition, 2012* 8. *Stuart Warren and Paul Wyatt, Organic synthesis, the disconnection approach, 2nd edition, Wiley, 2012.*
REFERENCE BOOKS	1. *W. Carruthares, Iain coldham, Modern Methods of Organic Synthesis South Asia Edition, Cambridge University Press, Fourth Edition, 2015.* 2. *F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry Part B: Reaction and Synthesis, Springer, 5th Edition, 2010.* 3. *J. March and M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edition, Wiley, 2013.* 4. *I. L. Finar, Organic Chemistry Vol. I & Vol. II, Longman (Cambridge), 2011.*
CH-513	**PHYSICAL CHEMISTRY III** **4 credits**
UNIT-I	***Exact Quantum Mechanical Results***
	The Schrodinger equation and the postulates of quantum mechanics, Elementary application of the Schrodinger equation, Particle in a box, Harmonic oscillators, Rigid rotator and hydrogen atom.
UNIT-II	***Approximate Methods & Angular Momentum***
	The variation theorem, Time independent perturbation of non-degenerate systems, Application of Variation Method and Perturbation Theory to the He atom. Ordinary angular momentum, generalized angular momentum, Eigen functions for angular momentum, Addition of angular momentum.
UNIT-III	***Chemical Bonding and Orbital Approximation Methods***
	LCAO-MO Theory, Born-Oppenheimer Approximation, The independent particle approximation, The π-electron separation approximation, Molecular Orbital Theory and its Applications, Valence Bond Theory and its Applications. Huckel's MOT and its Chemical Applications, The extended Huckel Method.
UNIT-IV	***Quantum Mechanical Treatment to Molecules***
	Molecular Geometry: Equilibrium Geometry, Potential Energy Surface, Geometry

	Optimization, Frontier Molecular Orbitals, Molecular Vibrational Frequencies, Thermodynamic Properties.
TEXT BOOKS:	*1. Introductory Quantum Chemistry, A.K. Chandra* *2. Introduction to Computational Chemistry by Frank Jensen, Wiley publication.* *3. Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Ed. Wiley & Sons, New York.* *4. Notes on Molecular Orbital Calculations by J.D. Roberts*
REFERENCE BOOKS:	*1. D. A. McQuarrie, Quantum Chemistry, Oxford University Press, 1983.* *2. I. R. Levine, Quantum Chemistry, Prentice Hall India (Ltd), 1995.* *3. The Chemical Bond: Fundamental Aspects of Chemical Bonding, Eds. Gernot Frenking, Sason Shaik; Wiley-VCH, 2014*
CH-514	**Analytical Techniques in Organic Chemistry** **4 credits**
UNIT-I	**Nuclear Magnetic Resonance**
	Magnetic properties of nuclei, Theory of magnetic nuclear resonance with special reference to proton, Instrumentation, Chemical shift, Simple spin-spin interaction, Shielding effects, Diamagnetic anisotropy, NOE, ^{13}C, ^{15}N, ^{19}F, ^{31}P NMR (preliminary idea).
UNIT-II	**Mass Spectrometry**
	Introduction, Mass spectrum, Determination of molecular formulae, molecular ions, Parent peak, Base peak, Use of molecular fragmentation, McLafferty rearrangement, Mass spectra of some classes of compounds (hydrocarbons, alcohols, phenols, ketones, aldehydes, acids and esters)
UNIT-III	**Spectroscopic Identification of Organic Compounds**
	Problems involving identification of organic compounds using UV, IR, NMR and Mass spectroscopy.
UNIT-IV	**Optical Rotatory Dispersion and Circular Dichroism**
	Plane polarized and circularly polarized lights, Circular birefringence and circular dicroism, ORD, Cotton effect, Rotatory Dispersion of ketones, the Octant rule, Axial haloketone rule.
TEXT BOOKS:	1. *Introduction to Spectroscopy by Donald L. Pavia, Gary M. Lampman, George S. Kriz, and James R. Vyvyan, Cengage Learning India Private Limited; 2015* 2. *R.M. Silverstein, G. C. Bassler, T. C. Morril, Spectrometric identification of Organic Compounds, John Wiley & Sons, Inc, 2010* 3. *D. Nasipuri, Stereochemistry of Organic Compounds Principles and Applications, New Age International Publishers, 3rd Edition, 2011* 4. *Spectroscopic Identification of Organic Compounds: Silverstein &Basselor, Wiley; 8th edition, 2014*
REFERENCE BOOKS	1. *Spectroscopy of Organic Compounds, by P S Kalsi, New Age International, 2007* 2. *Basic ^{1}H- and ^{13}C NMR spectroscopy, by M. Balci, Elsevier, 2005*
CH-515	**PHYSICAL CHEMISTRY PRACTICAL** **2 credits**
	1. Determination of ionization constants of weak acids and verification of Oswald's Dilution law. 2. Conductometric titration of a mixture of HCl+CH_3COOH with NaOH 3. Base hydrolysis of ethylacetateconductometrically. 4. Potentiometric titration of strong acid with strong base. 5. Verification of Beer's Lambert Law and unknown concentration determination. 6. Simultaneous estimation of Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$. 7. To estimate metal ions by spectrophotometric titration. 8. Determine the pK value of an acid-base indicator. 9. Determination of rate constant of acid hydrolysis of ethyl acetate. 10. Determination of unknown dextrose solution by polarimetry 11. Study of inversion of cane sugar in acid medium by polarimetry. 12. Adsorption of CH_3COOH on activated charcoal and verification of Freundlich's &Langumir's adsorption isotherm. 13. Determination of association constants of CH3COOH by distribution method between water and toluene. 14. To study the rate of acid catalysed iodination of acetone in presence of excess acid and acetone. 15. Determination of ionisation constants of multibasic acid using a pH meter.

Books:	1. *Practical Physical Chemistry by B. Viswanathan & P. S. Raghavan, Viva Books* 2. *Experimental Physical Chemistry by R.C. Das&B. Behera, McGraw-Hill Education*	
CH-516	**COMPUTATIONAL CHEMISTRY PRACTICAL**	**2 credits**
	1. Use of Microsoft Excel: Balancing Chemical Equations, Bond Enthalpy of Hydrocarbons, Spectrophotometric Analysis, Curve Fitting 2. Use of Chemdraw: Design molecular 2-D geometry, Preparation of reaction scheme 3. Execution of the Software to solve problems: Eigenvalues and Eigenvectors, Charge Density, Delocalization energy, Molecular geometry, Vibrational frequencies	

FOURTH SEMESTER
(Core Courses)

CH -521	**ADVANCED ORGANOMETALLIC CHEMISTRY**	**4 credits**
UNIT-I:	**σ- and π-Bonded Organometallic Compounds**	
	History and perspective, definition of organometallic compound, classifications, nature of metal-carbon bond, nomenclature, the 18-electron rule, σ-bonded organometallic compounds, transition metal π-complexes of olefinic, acetylenic, allylic, acyclic- and cyclic butadiene systems, sandwich compound, synthesis and reactivity of ferrocene, Davis-Green-Mingos (DGM) rule.	
UNIT-II:	**Fluxionality and Unique Reactions**	
	Stereochemical non-rigidity in allyl-, allene-, η^1-Cp and η^5-Cp complexes; concept of coordinative unsaturation, oxidative addition, cyclometallation, ortho-metallation, reductive elimination, insertion reaction, migratory insertion, deinsertion reaction, mechanistic aspects of CO insertion into $CH_3Mn(CO)_5$, intramolecular hydrogen transfer reaction, agostic interaction.	
UNIT-III:	**Organometallic Compounds in Catalysis**	
	General idea of catalysis, turnover number(TON), turnover frequency (TOF), hydrogenation of alkenes, Tolman catalytic loop, hydroformylation of alkenes (using cobalt and rhodium catalyst), enantioselective hydrofomylation, wacker process, mosanto acetic acid synthesis, Cativa process, hydrosilylation reactions, Zeigler-Natta polymerization of olefins, reduction of carbon monoxide by hydrogen (Fischer-Tropsch reaction), preliminary idea about the Pd-catalyzed cross-coupling reactions.	
UNIT-IV:	**Neutral Spectator Ligands and Alkene Metathesis Reactions**	
	Steric and electronic structure of phosphene, basicity of phosphene, monodentate and multidentate phosphines, N-heterocyclic carbenes (NHC), synthesis of NHC, alkene metathesis, mechanism of alkene metathesis, classification of metathesis reactions, significance of metathesis reactions.	
TEXT BOOKS:	1. *Basic organometallic Chemistry by B. D. Gupta, A. J. Elias, University Press (India) Pvt. Ltd., 2nd edn, Hyderabad, 2013* 2. *Organometallic Chemistry by R. C. Mehrotra, A. Singh, New Age International Ltd., 1st edn, 2011, New Delhi* 3. *Organometallic Compounds by Indrajeet Kumar, 4th edn, 2013, Pragati Prakashan, Meerut.* 4. *Inorganic Chemistry by G. L. Miessler, D. A. Tarr, 3rd edn., 2004, Pearson Education, Inc.*	
REFERENCE BOOKS	1. *Modern Aspects of Inorganic Chemistry by Emelius and Sharpe* 2. *Principle of Organometallic Chemistry by Coutes, Green, Powell and Wade* 3. *Organometallic Chemistry by Pauson*	

(Elective Courses)

CH-522	**ADVANCED ORGANIC SYNTHESIS**	**4 credits**
UNIT-I	**Chemistry of Heterocyclic Compounds I**	
	Synthesis, characterizations and applications of coumarins, quinazoline, phthalazine, cinnolenes and quinoxalines.	
UNIT-II	**Chemistry of Heterocyclic Compounds II**	
	Preparation and uses. Hantzsch-Widman nomenclature of heterocyclic compounds. General approach to heterocyclic synthesis-cyclisation and cycloaddition route. Synthesis and reactions of common heterocyclic compounds containing imidazole,	

	pyrazole, pyrimidine rings.	
UNIT-III	**Applications of Organometallic Reagents in Organic Synthesis**	
	Organometallic reagents, Preparation, structural and characteristic aspects: oxidative insertion, reductive elimination, ligand migration from metal to carbon. Organo lithium, organo copper compounds, organo boranes, organometallic compounds of Zinc, Cadmium, nickel, palladium, mercury and their utilization in chemical reactions.	
UNIT-IV	**Modern Synthetic Methods**	
	Reactions involving triple bond (Sonogashira reaction), C-C (Kumada, Negishi, Heck, Suzuki and Stille reactions) and C-N (Buchwald-Hartwig reaction) cross-coupling reaction. Protection and deprotection of functional groups (R-OH, R-CHO, RCO-R, R-NH_2 and R-COOH).	
TEXT BOOKS	*1. Organic Chemistry II by I. L. Finar* *2. Principles of Organic Synthesis by R. O. C. Norman* *3. Creativity in Organic Synthesis by J. S. Bindra and R. Bindra* *4. Heterocyclic Chemistry by A R Katrizsky* *5. Recent Literatures and Reviews*	
REFERENCE BOOKS	*1. Jonathan Clayden, Nick Greeves, and Stuart Warren. "Organic Chemistry," Oxford University Press, 2014.* *2. The Essence Of Heterocyclic Chemistry, Parikh, Arun, New Age International, 1st Edition, 2013* *3. Heterocyclic Chemistry, V. K. Ahluwalia, Alpha Science International, 2012* *4. Advanced Organic Chemistry: Structure and Mechanisms (Part A &B). Frances A Carey and Richard J Sundberg, Springer, 2015* *5. Heterocyclic chemistry, R. K. Bansal, New Age International Private Limited; Fifth edition, 2017.*	
CH-522	**ADVACED ANALYTICAL CHEMISTRY**	**4credits**
UNIT-I:	***Reliability of Analytical Data***	
	Errors in chemical analysis, classification of errors, significant figures, precision andaccuracy, methods of expressing accuracy, absolute error and relative error, methodsof expressing precision, average deviation, standard deviation, confidence limits,median value, range, coefficient of variation. Sampling in analysis definition: Theory ofsampling, technique of sampling, statistical criteria of good sampling and required size,stratified sampling, transition and storage samples.	
UNIT-II:	***Ultraviolet and Visible Spectrophotometry***	
	Introduction, nature of absorbing species, visual colorimetry, photo-electric cell andfilters, Photoelectric filter photometry, errors in photoelectric photometry,Spectrophotometry, working of spectrophotometer, simultaneous spectrophotometry,differential spectrophotometry, reflectance spectrophotometry, photometric titrations,composition of coloured complex Sandell's sensitivity, relative concentration and Ringbon's plot.	
UNIT-III:	***Electron Microscopy***	
	Introduction to optics, Principles of image formation, Light microscopy techniques, Electron Microscopy (SEM and TEM), Instrumentation of SEM and TEM, Application of SEM and TEM, Limitations of electron microscopy	
UNIT-IV	***Analytical Applications of Organized Assemblies***	
	Basic concepts of organized assemblies, Application of micellar systems for UV-Visible/fluorescence spectroscopic detection of ions, micellar enhanced phosphorescence and fluorescence, micellar systems in liquid-liquid extraction, surfactant aggregates in flame and plasma atomic spectrometry, micellar systems in chromatography, recent developments in micellar chromatography, application of surfactants in gel electrophoresis.	
TEXT BOOKS	*1. Basic Principle of Analytical Chemistry by S.M. Khopkar* *2. A Text Book of Quantitative Inorganic Analysis by A.I. Vogal.*	
REFERENC	*1. Physical Chemistry of Macromolecules by C. Tanford*	

E BOOKS		
CH-522	**PHOTOPHYSICAL CHEMISTRY**	**4 Credits**
UNIT-I:	***Mechanism of Absorption and Emission of Radiation of Photochemical Interest***	
	Importance of photochemistry, Laws of photochemistry, photochemistry and spectroscopy, Interaction between light and matter, electronic energy states of atoms, spectroscopic terms for electronic states, orbital symmetry and molecular symmetry, and notation for excited states of organic molecules, Electric dipole transition, Einstein's treatment absorption and emission phenomena, time-dependent Schrödinger equation, the rules governing the transitions between two energy states, Nature of changes on electronic excitation, Electronic, vibrational and rotational energies, potential energy diagram, shapes of absorption band and Frank-Condon principle, emission spectra, environmental effect on absorption and emission spectra, excited state dipole moment, excited state acidity constants-pk^* values, and Wigner spin conservation rule.	
UNIT-II:	***Photophysical Kinetics of Uni and Bimolecular Processes***	
	Types of photophysical pathways, radiationless transitions-internal conversion and intersystem crossing, fluorescence emission, delayed fluorescence, Quenching of Fluorescence, Theory of Collisional Quenching, Derivation of the Stern-Volmer Equation, Theory of Static Quenching, Combined Dynamic and Static Quenching, Examples of Static and Dynamic Quenching, Deviations from the Stern-Volmer Equation, Quenching Sphere of Action, Derivation of the Quenching Sphere of Action, Effects of Steric Shielding and Charge on Quenching, Fractional Accessibility to Quenchers, Applications of Quenching to Proteins and Membranes, Characteristics of Resonance Energy Transfer, Theory of Energy Transfer for a Donor–Acceptor Pair, Distance Measurements Using FRET.	
UNIT-III:	***Fluorophores***	
	Intrinsic or Natural Fluorophores, Extrinsic Fluorophores, Red and Near-Infrared (NIR) Dyes, DNA Probes, Chemical Sensing Probes, Special Probes. Green Fluorescent Protein, Other Fluorescent Proteins, Long-Lifetime Probes, Proteins as Sensors	
UNIT-IV:	***Instrumentations***	
	Principles & techniques of Steady State Spectrofluorometers & TCSPC Spectrofluorometers and its Applications, brief concept and applications of Fluorescence Anisotropy & Fluorescence lifetime.	
Text Book	1. *Fundamentals of Photochemistry by K. K. Rohatagi-Mukherjee* 2. *Principles of Fluorescence Spectroscopy by J. R. Lakowicz*	
Reference Book	1. *Molecular Photochemistry by N. J. Turro,* **2.** *Principles of Photochemistry by J.A. Baltrop& J.D. Coyle*	
CH-523	**CHEMISTRY OF NANO MATERIALS**	**4credits**
UNIT-I:	**Semiconductors and Devices**	
	Conducting and semiconducting organic materials. Synthesis and characterizations of organic semiconductors, Conducting and semiconducting materials and insulator, Band gap engineering. Doping of semiconductors. Application of carbon-based materials. Electronic devices and coating.	
UNIT-II:	**Nanomaterials for Energy Conversion and Storage Materials**	
	Nanomaterials for Solar Energy Conversion Systems. Principles of photovoltaic energy conversion (PV), Structural characteristics and concepts. Types of photovoltics Cells, Physical concept of photovoltaic cells, Organic solar cells, Dye-Sensitized Solar Cells, Organic-Inorganic Hybrid solar cells. Device fabrication techniques and characterizations, Applications of nanomaterials in in agriculture, food, textile, cosmetics. Current status and future trends.	
UNIT-III:	**Nanostructured Materials**	

	Intermolecular forces during the formation of nanostructured materials, Structure and features of conducting and ferroelectric materials, structure and features of ferroelectric materials, dielectric properties, piezo and inverse piezoelectric effects, ceramic materials, organic/inorganic hybrid materials and their fabrications and applications.	
UNIT-IV	**Polymers and their Applications**	
	Stress-strain behavior, High temperature resistant organic/inorganic polymers, effect of chain flexibility and other steric factors, entropy and heat of fusion, glass transition temperature, relationship between Tm and Tg. Effect of molecular weight on polymer properties and their applications. Synthetic procedure commercial polymers (polycarbonate, polyurethane, polymethylmethacrylate, polyethyleneterpthalate, Nylon, polystyrene), Fire retarding and biomedical polymers	
TEXT BOOKS	1. *Organic Photovoltaics – Materials, Device Physics and Manufacturing Technologies, (eds. C. Brabec, V. Dyakonov, U. Scherf), 2nd Ed., Wiley-VCH, Germany, 2014.* 2. *Solar cells: Operating principles, technology and system applications by Martin A Green, Prentice Hall Inc, Englewood Cliffs, NJ, USA, 1981.* 3. *Semiconductor for solar cells, H J Moller, Artech House Inc, MA, USA, 1993.* 4. *Recent Literatures and Reviews*	
REFERENCE BOOKS	1. *Solis state electronic device, Ben G Streetman, Prentice Hall of India Pvt Ltd., New Delhi 1995.*	
CH-523	**SUPRAMOLECULAR CHEMISTRY**	**4credits**
UNIT-I	***Fundamentals of Supramolecular Chemistry***	
	Terminology and definitions in supramolecular chemistry. Intermolecular forces: Ion pairing, ion-dipole and dipole-dipole interactions; hydrogen bonding; cation-pi, anion-pi, pi-pi interactions and Van der Waal forces. Solvent and solution properties, solvation and hydrophobic effect. Binding constants; definition and use, determination of binding constant by physical methods.	
UNIT-II	***Molecular Recognition***	
	Principle of molecular recognition, host-guest complementarity, preorganisation, chelate effect, cooperativity. Structure and function of receptors with molecular clefts, Synthesis and applications of supramolecular host with multiple hydrogen bonding sites (crown ethers, lariat ethers, podands, cryptands, spherands, calix[n]arenes, cyclodextrine, ionophores) as cation and anion binding receptors and receptors for ion-pair recognition.	
UNIT-III	***Reactivity and Catalysis***	
	Organocatalysis mediated through hydrogen bonding, preconcentration, self-assembly of catalysts and preorganisation of catalyst-substrate systems. Influence of organisation (effective molarity) on catalysis, Catalytic acyl transfer, acid-base catalysis, catalysis hydrolysis as ATPase mimic.	
UNIT-IV	**Applications of Supramolecular Materials**	
	Basic principles and applications, Covalent organic frameworks, Metal organic frameworks, Host-guest complexation, micelles, polymers, Multifunctional catalysis.	
TEXT BOOKS:	1. *Supramolecular Chemistry: from Molecules to Nanomaterials Eds. by P.A. Gale and J.W. Steed (2012).* 2. *Modern Supramolecular Chemistry by F. Diederich, P. J. Stang, R. T. Tykwinski (2008). .* 3. *Core Concepts in Supramolecular Chemistry and Nanochemistry by J. W. Steed, D. R. Turner, K. J. Wallace (2007).* 4. *Supramolecular Chemistry by J.W. Steed and J.L. Atwood (2011).* 5. *Supramolecular Chemistry: Concepts and Perspectives by J.-M. Lehn, Wiley VCH, Weinheim (1995).* 6. *Recent Literatures and Reviews*	
REFRENCE	1. *Supramolecular Chemistry by V. Balzani (Editor), L. De Cola, Kluwer, Dordrecht*	

BOOKS:	*(1992).* 2. *Introduction to Supramolecular Chemistry by H. Dodziuk, Kluwer Academic Publishers, The Netherlands (2002).* 3. *Supramolecular Assemblies Y. Murakami (Editor), Mita Press, Tokyo, (1990).* 4. *Advances in Supramolecular Chemistry, Vol 1 (1990), Vol 2 (1992), Vol 3 (1993) by G. W. Gokel (Editor), JAI Press, Greenwich.* 5. *Supramolecular Chemistry – Fundamentals and Applications. Advanced Textbook by T. Kunitake, K Ariga, Berlin: Springer-Verlag Heidelberg, 2006. 208 p. ISBN 978-3-540-01298-6.*	
CH-523	**MOLECULAR MODELING**	**4credits**
UNIT-I	***Ab initio and Density Functional Treatment of Molecules***	
	The Born - Oppenheimer Approximation, Ab initio methods, Density Functional Methods, Basis sets and basis functions, Optimizations of Molecules, Convergence criteria, Computation of Solvation	
UNIT-II	***Spectral and Electronic Properties of Molecules***	
	Population analysis, Molecular electrostatic potential and atomic charges, Molecular vibrational frequencies, Thermodynamic properties	
UNIT-III	***Visualization and Dynamics of Macromolecules***	
	Structure representation: Building of small molecules, co-ordinate system for structure representation, Building of Biopolymers and oligopeptides, Conformational analysis, Molecular Docking, Molecular Mechanics approach, Molecular Dynamics Method, Visualization of macromolecules using application programs	
UNIT-IV	***Computational Design on Drugs and Functional materials***	
	Molecular Interactions and recognitions, Enzyme Inhibition Reactions, Protein folding, DNA-Adduct, Structure and features of conducting and semiconducting organic materials, Substituent effects on functional organic materials, Machine Learning approach as future prospect.	
TEXT BOOKS:	*Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Ed. Wiley & Sons, New York.* *Introduction to Computational Chemistry by Frank Jensen, Wiley publication.* *Andrew R. Leach, Molecular Modeling: Principles and Applications, 2nd Ed., Prentice Hall, 2001.*	
REFRENCE BOOKS:	*I. R. Levine, Quantum Chemistry, Prentice Hall India (Ltd), 1995.* *D. A. McQuarrie, Quantum Chemistry, Oxford University Press, 1983.*	
CH-524	**PROJECT**	**4 credits**
	Each student shall carry out project work under the supervision of one or more mentor(s) in the School of Chemistry, Sambalpur University. Duration of the work shall be twelve weeks (approximately 200 hours). The findings of the project work should be submitted in the form of a dissertation for evaluation by a Board of Examiners. *The project work will be assigned at the beginning of 3rd semester.*	
CH-525	**COMPREHENSIVE VIVA**	**2 credits**
	Comprehensive viva-voce examination shall be conducted jointly by the external and internal Examiners. Short questions on the theoretical principles, experimental methodologies and instrumentations etc. of the different experiments included in the entire practical/project syllabus of semesters-I, -II, -III and -IV may be asked.	
CH-526	**SEMINAR**	**2 credits**
	Each student has to present a seminar on published paper in the last two years.	