COURSES OF STUDY FOR THE M. Sc. EXAMINATION IN CHEMISTRY

DEPARTMENT OF CHEMISTRY
VSS UNIVERSITY OF TECHNOLOGY (FORMORLY UCE)
Burla - 768 018

SEMESTER SYLLABUS
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<tr>
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# Elective Courses for 3rd and 4th Semesters

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<td>Supramolecular Chemistry</td>
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<td>MCH-217</td>
<td>Biocatalysis for Industry, Medicine and Environment</td>
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<td>MCH-218</td>
<td>Bioinorganic Chemistry</td>
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<tr>
<td>MCH-219</td>
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DETAIL COURSE

FIRST SEMESTER

MCH-101: GROUP THEORY AND QUANTUM CHEMISTRY  4 Credits

UNIT-I: GROUP THEORY
Symmetry elements and symmetry operations, matrix representation of symmetry operation, classes of operations, point groups, C_n, C_n v, C_nh, S_n, D_n, D_n d, D_{nh}, T_d, O_h, D_{x, v}, C_{x, v} and D_{x, h}, properties of point groups, group theoretical representations, Orthogonality theorem, construction of character tables for C_2 v, C_3 v, T (cubic), C_4 (cyclic) and D_{x, h} groups, projection operator and direct product.

UNIT-II: WAVE MECHANICS OF SOME SYSTEMS
Application of Schrödinger wave equation to Hydrogen atom, transformation of co-ordinates, separations of variables, the \( \phi \)-equation, the \( \theta \)-equation and the R-equation and their solutions, spherical harmonics, the shapes of s, p & d-orbital probability density in 1s-orbital, physical interpretation of the Hydrogen orbitals, space quantisation on electronic orbits, the radial distribution function and radial distribution curves, mutual interaction of electron orbitals and resultant vectors, Russel-Saunders's coupling \( j-j \) coupling, ground state term symbols and Hund’s rule, micro states and derivation of Russell-Saunders’s term for \( P^2 \), \( d^2 \) and pd configuration.

UNIT-III: APPROXIMATION METHOD
The variation theorem and it’s application to Hydrogen atom in derivation of its ground state energy, the secular equations, the LCAO approximation (molecular orbital theory) and it’s application to Hydrogen molecule ion, bonding and anti bonding orbitals, electron distribution in Hydrogen molecule ion, stability of Hydrogen molecule ion, the valence bond approximation and application to the Hydrogen molecule, symmetric and anti symmetric energy levels, the Classical interaction energy, resonance and contribution to ionic terms, anti symmetric nature of overall wave function (Pauli’s Exclusion Principle).

BOOKS:
1. Group Theory : F.A. Cotton
2. Theoretical Inorganic Chemistry : Day and Selbin
3. Introduction to Quantum Chemistry : A.K. Chandra

MCH-102: COORDINATION CHEMISTRY  4 Credits

UNIT-I: THEORIES OF METAL-LIGAND BONDING:
Crystal field theory: Important aspects of crystal field theory -d-orbitals splitting in octahedral, tetrahedral and square planar complexes - 10Dq value and its calculation - CFSE in weak field and strong field cases - Factors affecting magnitude of 10Dq - Spectrochemical series - Jahn-Teller
Theory & applications of crystal field theory (colour and magnetic properties of complexes) - Limitations of crystal field theory.

**Molecular Orbital theory**: Nephelauxetic effect - MO energy level diagrams for octahedral, tetrahedral and square planar complexes, Measurement of pi-bonding effects.

**UNIT-II STUDY OF COMPLEXES IN SOLUTION:**

**UNIT-III ELECTRONIC SPECTRA OF METAL COMPLEXES:**
Spectra of transition metal ions - Term symbols of dn ions – Orgel diagrams for dn ions and Tanabe - Sugano diagrams for dn ion complex - charge transfer transitions - Selection rules and transition probabilities based on symmetry considerations.

**UNIT-IV MAGNETIC PROPERTIES OF COMPLEXES:**
Types of magnetism (dia, para, ferro and anti ferromagnetism) - Temperature independent paramagnetism - Magnetic susceptibility and its determination by Gouy and Faraday methods - Calculation of magnetic moment from magnetic susceptibility - Spin-orbit couplings and its effect on magnetic moments - orbital contribution to magnetic moment-single molecule magnets.

**UNIT-V KINETICS AND MECHANISMS OF REACTIONS:**
Inert and labile complexes-substitution reactions in octahedral and square planar complexes - D, Id, IA and A mechanisms – Bond making and Bond breaking - The Langford- Gray nomenclature- Coordination number and substitution mechanisms- Stereochemistry of substitution- Effect of nonparticipating ligands on the stability of complexes. Trans-effect in square – planar complexes - Theories of Trans-effect (Polarization and pi-bonding theories)- Quantitative aspects of the Trans effect-Dissociation mechanism- Substitution of non-coordinating and coordinating solvents - Electron transfer reactions: Inner and outer sphere mechanisms - Marcus Cross relationship - Template effect.

**BOOKS:**
7) Molecular Magnetism by O.Kahn, Wiley VCH,1993
REFERENCE BOOKS:

MCH-103: STRUCTURE AND REACTIVITY 4 credits

UNIT-I: NATURE OF BONDING IN ORGANIC MOLECULES
Delocalized chemical bonding, conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel’s rule, energy levels of pi-molecular orbitals of simple systems, annulenes, anti-aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent-addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

UNIT-II: REACTION MECHANISM: STRUCTURE AND REACTIVITY
Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond’s postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, Hard and soft acids and bases. Effect of structure on reactivity: resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

UNIT-III:
(a) REACTION INTERMEDIATE
Non-classical carbocations, Free radicals, Carbenes, Nitrenes, Arynes.
(b) GENERAL DISCUSSION ON THE FOLLOWING:
Solvent effect, Isotope effect, Kinetic salt effect, Stereoselective, Regioselective, Stereospecific and Regiospecific reactions, Stereo electronic factors in Transition State stability.
**BOOKS:**
1. Advanced organic chemistry: Reaction mechanism and structure: Jerry March (Wiley Eastern Limited)
2. Physical basis of organic chemistry : N.Isaac (Wiley Eastern Limited)

**MCH-104: STEREOCHEMISTRY**

**4 credits**

**UNIT-I:**
Chirality, Fischer projection and R and S notations, Threo and erythro nomenclature, E and Z nomenclature, Optical isomerism in biphenyils and allenies, Concept of Prostereoisomerism and Assymetric synthesis (including enzymatic and catalytic nexus), Conformation of a few acyclic molecules (alkanes, haloalkanes), Conformation of cyclic systems having one and two sp2 carbon atoms.

**UNIT-II:**
Dynamic stereochemistry: Conformation and reactivity, Selection of substrates, Quantitative correlation between conformation and reactivity, (Weinsteinei-Eliel equations and Curtin-Hammett principles), Conformational effects on stability and reactivity in acyclic compounds (ionic elimination, intramolecular rearrangements, NGP) and in cyclic systems, (Nucleophilic substitution reaction at ring carbon, Formation and Cleavage of epoxide rings, Addition reactions to double bonds, Elimination reactions).

**UNIT-III:**
Molecular dissymmetry and chiroptical properties, linearly and circularly polarised lights, circular birefringence and circular dicroism, ORD, Plane curves, Cotton effect, Rotatory Dispersion of ketones, the Axial Haloketone rule, the Octane rule, Helicity rule, Lowe’s rule, Emperical rule involving the benzene chromophore.

**BOOKS:**
2. Stereochemistry : Kalsi
3. Stereochemistry : Elliel

**MCH-105: THERMODYNAMICS & ELECTROCHEMISTRY**

**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: NON-EQUILIBRIUM THERMODYNAMICS
Microscopic reversibility, entropy productions and irreversible process,
Different types of forces and fluxes, Stationary states,
Phenomenological equations, Onsager reciprocity theorem, Oscillatory
reactions.

UNIT-III: THERMODYNAMICS OF LIVING SYSTEMS
Bioenergetics and thermodynamics, Phosphate group transfer and ATP,
Biological oxidation-reduction reactions.

UNIT-IV: ELECTROCHEMISTRY
Interionic attraction theory and Debye-Huckel treatment, Derivation of
Onsager limiting law and its verification and modification, Activities,
activity coefficients, Debye-Huckel treatment, Debye-Huckel-Bronsted
equation, Salt effect, Determination of activity coefficients from
solubility method, Ion association, Determination of thermodynamic
dissociation constant of weak electrolytes by Shedlovsky method and by
EMF method, Aminoacid, hydrogen ion concentration, Ampholytes,
Isolelectric points.

UNIT-V: CHEMICAL KINETICS
Theories of reaction rates, Collision theory, Transition state theory of
uni and bimolecular reactions, Lindemann mechanism. Arrehenius and
activated complex, Reaction between ions, Salt effect, Steady-State
Kinetics, Kinetic and Thermodynamic concept of Reactions, Dynamic
chain (H₂ + Br₂ reaction, pyrolysis of CH₃CHO, Decomposition of
ethane) reactions.

UNIT-VI: FAST REACTIONS
General feature of Fast reactions, Study of Fast reactions by relaxation,
Stopped flow, Flash photolysis and NMR techniques.

BOOKS:

2. Physical Chemistry : D.N. Bajpai
3. Physical Chemistry : A.W. Atkins
4. Physical Chemistry Through Problems : Dogra & Dogra
5. Physical Chemistry Principles & Problems : Jain & Jabuhar
7. Thermodynamics for Chemists : S. Glasstone
8. Thermodynamics for Irreversible Processes : S. Hasse
9. Thermodynamics for Irreversible Processes : L Prigogine
11. Electrochemistry: S. Glasstone
13. Chemical Kinetics: Frost & Pearson
15. Chemical Kinetics: K.J. Laidler

REFERENCE BOOKS:
3) Principles of colloids and surface chemistry, 2nd edition, P.C. Hiemenz. Marcel Dekker, INC.
   1986.
   1997.
5) Introduction to Thermodynamics of Irreversible Processes by I.Prigogine, 3rd Ed. Interscience

MCH-191: INORGANIC GENERAL PRACTICAL 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.

MCH-192: ORGANIC GENERAL PRACTICAL-I 2 Credits
Isolation and identification of compounds in a mixture of two organic compounds. IR spectra to be used for confirmation of functional groups.

SECOND SEMESTER

MCH-106: ANALYTICAL CHEMISTRY 4 Credits

UNIT-I: RELIABILITY OF ANALYTICAL DATA
a. Errors in chemical analysis, classification of errors, significant figures, precision and accuracy, methods of expressing accuracy, absolute error and relative error, methods of expressing precision, average deviation, standard deviation, confidence limits, median value, range, coefficient of variation.
b. Sampling in analysis definition: Theory of sampling, technique of sampling, statistical criteria of good sampling and required size, stratified sampling, transition and storage samples.

UNIT-II: SOLVENT EXTRACTION AND ION EXCHANGE
a. Solvent extraction: basic principles, classification of extraction, mechanism of extraction, extraction equilibria, technique of extraction, applications in analytical chemistry.

b. Ion exchange: synthesis and characteristics of ion exchange, ion exchange equilibria, technique of ion exchange, application of ion exchange for separation.

UNIT-III: Ultraviolet and visible spectrophotometry: Introduction, nature of absorbing species, visual colorimetry, photo-electric cell and filters, 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.

BOOKS:

REFERENCE BOOKS:
2) Perspectives in Modern Chemical Spectroscopy by D.L.Andrews Springer verlag, 1990
MCH-107: SPECTROSCOPY-I  
4 Credits

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 AND ROTATIONAL SPECTROSCOPY
Molecular Spectra of Diatomic Gases, Classification of molecules, Rotational Spectra, Vibrational Spectra, Vibrational-Rotational Spectra, P, Q and R Branches

UNIT-III: RAMAN SPECTROSCOPY
Theory of Raman spectra, Rotational Raman spectra, Vibrational Raman spectra, Rotational-Vibrational Raman spectra, comparison with IR spectra.

BOOKS:
2. Physical Chemistry : D.N. Bajpai
3. Physical Chemistry : A.W. Atkins
4. Physical Chemistry Through Problems : Dogra & Dogra
5. Physical Chemistry Principles & Problems : Jain & Jabuhar
6. Statistical Thermodynamics : M. C. Gupta
7. Fundamentals of Statistical Mechanics : B.B. Laud
10. Fundamentals of Molecular Spectroscopy : G.M. Barrow

MCH-108: ORGANIC REACTION MECHANISM  
4 credits

UNIT-I:
The S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanisms. The neighbouring group mechanism, Neighboring group participations by sigma and pi bonds, anchimeric assistance. Classical and nonclassical carboxations, phenonium ions, norbornyl system, common carbocation rearrangements, application of NMR spectroscopy in the detection of carboxations. The S_N1 mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis, ambident nucleophile, regioselectivity.

UNIT-II:
(a) Aliphatic Electrophilic Substitution mechanism: S_E1, S_E2 and S_E1 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).
(b) Aromatic electrophilic substitution mechanism: Structure reactivity relationship in mono-substituted benzene, ring isomer proportions, orientation in benzene ring with one or more than one substituent, Orientation in other ring systems, Vilsmeir - Haack reaction, Pechmann reaction.

UNIT-III:

(a) Aromatic Nucleophilic Substitution mechanism: Introduction, to different mechanisms, Aromatic nucleophilic substitutions (SNAr, SN1 aryne), Effect of substrates, leaving groups, and nucleophile, Reactions: Nucleophilic displacement in areno-diazonium salts by different nucleophiles, Chichibabin reaction.
(b) Free radical Substitution: Reaction at sp² carbon, Reactivity in aliphatic substrates, Reactivity at bridge head position, Reactivity in aromatic substrates.

UNIT-IV:

(a) Addition to carbon-carbon multiple bonds, Electrophilic, Nucleophilic and Free radical addition, Orientation and Reactivity, Addition to cyclopropanes, Reactions: Hydroboration, Michael reaction, Sharpless Asymmetric epoxidation.
(b) Addition to carbon-heteroatom multiple bonds: Mechanism and reactivity, Reactions: Mannich reaction, LiAlH₄ reduction of carbonyl compounds, acids, esters, nitriles, addition of Grignard reagents - Reformatsky reaction, Aldol condensation, Knoevenagel condensation, Perkin reaction, Tollens reaction, Wittig reaction, Prins reaction, Benzoin condensation.

UNIT-V:


UNIT-VI: REARRANGEMENTS

General mechanistic considerations – nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements:

BOOKS:
1. Advanced organic chemistry: Reaction mechanism and structure : Jerry March (Willey Eastern Limited)
2. Organic reaction mechanism: Kalsi,
Step Polymerisation:

Radical Chain Polymerisation:
Nature of radical chain polymerisation - Rate of radical chain polymerisation - initiation - molecular weight - chain transfer - inhibition and retardation - determination of absolute rate constants - energetic characteristics - auto acceleration.

Emulsion polymerisation:
Qualitative picture - quantitative aspects - other characteristics of emulsion polymerisation.

Ionic chain polymerisation:
Comparison of radical and ionic polymerisations - kinetics - cationic polymerisation of the carbon - carbon double bond - Anionic polymerisation of the carbon - carbon double bond - Block copolymers.

Chain copolymerisation:
Copolymer composition - radical co-polymerisation - ionic co-polymerisation - kinetics of copolymerisation, Applications of co-polymerisation.

Ring opening polymerisation:
General characteristics - Cyclic ethers - Cyclic amides.

Stereochemistry of polymerisation:
Types of stereo isomerism in polymers - Properties of stereo regular polymers - forces of stereoregulations in alkene polymerisation, Ziegler-Natta polymerisation of non-linear vinyl polymers - kinetics

Polymer structure and physical properties:
Crystalline melting point - Glass transition - properties involving large deformations - properties involving small deformations - property requirements and polymer utilisations.

Mechanical behaviour of polymers:

BOOKS:
REFERENCE BOOKS:

MCH-110: SURFACE CHEMISTRY & NUCLEAR CHEMISTRY 4 Credits

SURFACE CHEMISTRY

UNIT-I: PHASE RULE AND CATALYSIS
A. Derivation of phase rule, Brief concept on one and two component system, Application of phase rule to three component systems of both solids and liquids.
B. Kinetics of Catalytic Reactions: Acid-base Catalysis, Enzyme Catalysis, Heterogeneous Catalysis.

UNIT-II: ADSORPTION

UNIT-III: MACROMOLECULES
Polymer-definition, Types of polymer, Number average and weight average macromolecules, determination of molecular weights of macromolecules (Osmometry, Viscometry, Diffusion and Light scattering method), Kinetics of polymerization, Donnan Effect, Stereochemistry of polymerization.

BOOKS:
2. Physical Chemistry : D.N. Bajpai
3. Physical Chemistry : A.W. Atkins
4. Physical Chemistry Through Problems : Dogra & Dogra
5. Physical Chemistry Principles & Problems : Jain & Jabuhar
7. Molecular Quantum Mechanics : P.W. Atkins
8. Notes on Molecular Orbital Calculations : J.D. Roberts

NUCLEAR CHEMISTRY
Classification of nuclides, nuclear stability, binding energy and nuclear models. Characteristics of radioactive decay, decay kinetics, parent-daughter decay growth relationships, detection and measurement of radioactivity, advances in the solid and liquid scintillation counting techniques, methods for the determination of half life period
of single and mixed radionuclides. Nuclear fission, nuclear fuels and nuclear reactors, nuclear fuel reprocessing, fast breeder reactors, radiological safety aspects and radioactive waste managements. Interaction of radiation with matter, effect of ionizing/non-ionizing radiations on water, aqueous solutions and on organic compounds, radiation dosimetry. Preparation and separation of radioactive isotopes, application of radioisotopes and radiations in various fields, isotopic dilution techniques, neutron activation analysis and its applications.

BOOKS:
3. R.T. Overman, Basic concept of Nuclear Chemistry, Chapman & Hall.

MCH-193: PHYSICAL GENERAL PRACTICAL 2 Credits
(Any Six from the Following)
1. Determination of ionization constants of weak acids and verification of Oswald's Dilution law.
2. Verification of Onsager's Limiting law.
3. Conductometric titration of a mixture of HCl+CH₃COOH with NaOH
4. Determination of solubility product of BaSO₄.
5. Potentiometric titration of strong acid with strong base.
6. Verification of Beer's Lambert Law and unknown concentration determination.
7. Verification of additivity rule spectrophotometrically.
8. Determination of temperature coefficient and energy of activation of hydrolysis of ethyl acetate.
9. To determine the rate constant of base hydrolysis of ester titrometrically.
10. To study the complex formation between ammonia and Cu⁺².
11. To study of an equilibrium KI + I₂ = KI₂.
12. To study the simultaneous equilibria in benzoic acid - benzene water system.
13. Determination of unknown dextrose solution by polarimetry
14. Study of inversion of cane sugar in acid medium by polarimetry.

BOOK:
Experimental Physical Chemistry : Das and Behera
MCH-194: ANALYTICAL CHEMISTRY PRACTICAL 2 Credits

1. SPECTROPHOTOMETRY
   (a) Determination of composition of a complex by Job’s method.
   (b) Determination of stability constant of a complex.

2. ION EXCHANGE METHODS
   (a) Determination of total cation concentration in a given sample of water.
   (b) Separation of Ni (II) & Co (II) in cation exchange column using Citrate buffer as a chelating agent.

3. POLAROGRAPHY
   Determination of half wave potential of Cd(II) ion in KCl solution and estimation of Cd ion in unknown solution containing 0.1M KCl.

4. QUANTITATIVE ANALYSIS OF ORES AND ALLOYS
   Analysis of cement/dolomite/brass.

BOOK:
1. Experimental Physical Chemistry By R. C. Das and B. Behera
2. Applied chemistry- Theory and practice by Virmani and Narula
3. B. Tech Practical Chemistry by Kar, Dash and Mishra

THIRD SEMESTER

MCH-201: MATERIAL AND ENERGY BALANCE 4 credits

UNIT-I: MATERIAL BALANCE
(b) Material Balances Involving Chemical Reactions, Definition of Terms, Electrochemical Reactions, Recycling, Parallel and Bypassing Operations, Metallurgical Applications

UNIT-II: ENERGY BALANCES

UNIT-III: STOICHIOMETRY AND UNIT OPERATIONS

BOOKS:
4. Modern Aspect of Inorganic Chemistry: Emelius and Sharpe

MCH-202: ENVIRONMENTAL CHEMISTRY  4 Credits

Air Pollution: Air pollutants - Air quality standards - Production, fate, effects and control of gaseous pollutants - Oxides of carbon, nitrogen and Sulphur - Organic air pollutants - photochemical reactions, photochemical smog, Green house effect, Acid rain and Ozone depletion.
Water Pollution: Water quality - Water pollutants (inorganic and organic) - Sources, fate, effects and controlling measures - Chemical speciation - Pollution by radionucleides - Biochemical oxygen demand-Chemical oxygen demand, Eutrophication, Biodegradation of pollutants.
Oils in fresh & marine water: Sources of oil pollution - chemistry and fate of hydrocarbons - oil in run off and ground water – biodegradation - effect on aquatic organisms and communities – treatment and disposal technology.
Soil Pollution: Soil pollutants (Inorganic, organic, pesticides, radionuclides) - sources and effects on nature and properties of soil, crops, plants and terrestrial animals.
**Values in Environment:** The philosophy and Technology of living in tune with with nature and its assete. Nature-A silent teacher Ecology-The Indian Approach

**BOOKS:**
4) Environmental Pollution by H.M.Dix., Wiley, 1981.

**REFERENCE BOOKS:**

**MCH-203: INDUSTRIAL PROCESSES**

**4 Credits**

**UNIT-I:**


**UNIT-II:**

(a) Oil based industries: Oils and fats: Solvent extraction of oils, hydrogenation of oil, use of oil in the manufacturing of soap, paints and varnishes.
(b) Surface active agents: classification and manufacturing of detergents used for cleansing purpose.
(c) Fermentation industries. A general discussion on fermentation conditions, manufacturing of penicillin.

**UNIT-III:**

Pesticides and Pharmaceutical industries: DDT manufacture, BHC manufacture, 2,4-D manufacture, parathion manufacture, Pharmaceutical industry.

**BOOKS:**
2. Industrial Chemistry. By B. K. Sharma
MCH-291:  INDUSTRIAL PRACTICAL                    2 Credits

1. Determination of percentage of purity of commercially available different N, P and K fertilizer.
2. Water analysis: (a) Residual chlorine in town supply water (b) Ammonia content of sewage water
3. Determination of acid value, saponification value and iodine value of different oils
4. Determination of chloride in bleaching powder.
5. Determination of flash point of a lubricating oil.
6. Determination of viscosity of a lubricating oil.

BOOKS:  1. B. Tech Practical Chemistry by Kar, Dash and Mishra
         2. Advanced physical practical by Gurtu.

MCH-292:  ENVIRONMENTAL CHEM PRACTICAL                2 Credits

1. Determination of alkalinity of water
2. Determination of dissolved oxygen in a sample of water.
3. Determination of COD
4. Determination of chloride content in a sample of water.
5. Determination of iron content in a sample of water.

BOOKS:  1. B. Tech Practical Chemistry by Kar, Dash and Mishra
         2. Applied chemistry- Theory and practice by Virmani and Narula

FOURTH SEMESTER

MCH-204:  COMPUTER APPLICATION IN CHEMISTRY          4 Credits

UNIT-I:  INTRODUCTION TO COMPUTERS
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 MS-DOS. Windows operating systems.

UNIT-II:  PROGRAMME DEVELOPMENT PROCESS
Algorithm, Flowchart, Decision-table, elements of high level programming languages. Input-output statements, conditional statements, control structure, concept of data file,
file operations like searching, storing, with reference to Basic. C++.Types of data, variable, input and output statement, loop, Nested loop, subscript variable.

UNIT-III:
PROGRAMME DEVELOPMENT PROCESS
a. Development of small computer codes involving simple formulae in chemistry, such as- Vander Waals equation, pH titration, Kinetics, Radiation decay.

b. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Huckel theory.

BOOKS:
1. Computational Chemistry : A.C. Norris
2. Microcomputer Quantum Mechanics: J.P. Killngbeck
3. Computer Programming in Fortran-IV: V. Rajaraman
4. An Introduction to Digital Computer design: Rajaraman & Radhakrishnan

MCH-295: PRACTICAL ON COMPUTER IN CHEMISTRY 2 Credits
1. Use of computer programmes like MS Word, EXCEL, Lotus, FOXPRO.
2. Execution of the Software to solve problems.
3. Development of small programmes for solving chemical problems.

BOOKS:
MCH-296: INDUSTRIAL REPORT 2 Credits
The candidate has to undergo industrial training and submit a training report.

ELECTIVE COURSES FOR 3rd AND 4th SEMESTERS

MCH-205: INSTRUMENTAL METHODS OF ANALYSIS 4 Credits
UNIT-I:
(a) Atomic absorption spectral methods: Principle, instrumentation, flame atomisation, hollow cathode lamp, applications of atomic absorption in qualitative and quantitative analysis.
(b) Flame photometric methods: Basic principle, instrumentation and application in qualitative analysis.
UNIT-II:
Polarography: Concentration polarisation and overvoltage, Principle of diffusion of ion, Cathodic discharge of ion, limiting current density and limiting diffusion current, thickness of diffusion layer, halfwave potential, Basic principle, Instrumentation, Theory of current-voltage
curve, Theory of diffusion current, The Ilcovich equation, Polarographic wave and half wave potential, Applications of polarography, Oscillographic polarography, tensametry, amperometric titration.

UNIT-III:
Thermal methods: Thermogravimetry (TG), instrumentation for TG and applications of TG, Differential Thermal Analysis (DTA), instrumentation of DTA and application of DTA.

BOOKS:
1. Instrumental Methods of Analysis: H. Willard, L. Merritt, J. Dean and F. Settle
1. Analytical Chemistry (Theory & Practice) : U.N. Dash

MCH-206: INDUSTRIAL POLLUTION AND ITS MANAGEMENT  4 Credits

UNIT-I: AIR POLLUTION AND ITS CONTROL
Concept of atmosphere, sources and classification of air pollutants, some important air pollutants (SO\textsubscript{x}, NO\textsubscript{x}, CO\textsubscript{2}, Fluoride, hydrocarbon etc.) and their effects (acid rain, photochemical smog, green house effect, ozone layer depletion), characterization of gas emission from some major industries (Steel, aluminium, paper, fertilizer and thermal power station), sampling, analytical and instrumental techniques used for air quality monitoring, ambient air quality and permissible limits, prevention and methods for control of air pollution.

UNIT-II: WATER POLLUTION AND ITS MANAGEMENT
Sources and classification of water pollutants (suspended solids, oil, heavy metals, radioactive materials, microorganism) and their effects.) Sampling, analytical and instrumental methods used for physical, chemical and biological characterization of waste water from major industries (Steel, pulp and paper, textile, tannery, sugar and fertilizer), standard water quality and permissible limit, control of water pollution by primary, secondary and tertiary methods and treatment options for some industrial (paper, textile, tannery, steel) waste water.

UNIT-III: SOLID WASTE POLLUTION AND MANAGEMENT
Sources and characterization of solid wastes, hygienic problem, different methods for solid waste disposal and management (Hug feeding, open
dumps, ocean dumping, sanitary land fillings, incineration and pyrolysis, composting, recycle and reuse).

**BOOKS:**

2. Environmental Chemistry, A. K. Dey

**MCH-207: BIOCHEMISTRY**

**UNIT-I:** AMINO ACIDS AND PROTEINS  
Classification and functions of amino acids and proteins, Chemical reactions of amino acids, alkali titration of amino acids, Synthesis of peptides, Primary, secondary, tertiary and quaternary structures of proteins.

**UNIT-II:** LIPIDS  
Classification and Function of lipids, Structural lipids in membranes, lipids with specific biological activities, Resolution and Analysis of lipids, Biological membrane and transport.

**UNIT-III:** NUCLEIC ACIDS  
Structure and Function of nucleotides and nucleic acids, Replication, Transcription and Translation processes, Sequencing of nucleic acids, Genetic code, Recombinant DNA.

**UNIT-IV:**  
(a) Enzymes: Functions, Enzyme kinetics, Mechanism of enzyme action, Regulatory enzymes.  
(b) Nitrogen metabolism: Overview, Biosynthesis of amino acids (Tryptophan, serine, proline), Biosynthesis and Degradation of nucleotides.

**UNIT-V:** CARBON METABOLISM  
(a) Citric acid cycle, Production of acetate, Reactions of the citric acid cycle, Regulation of the citric acid cycle.  
(b) Oxidation of fatty acids, Digestion, Mobilization and Transport of fatty acids, β-oxidation.

**UNIT-VI:**

Oxidation and Photophosphorylation: Mitochondrial electron flow, ATP synthesis coupled to respiratory electron flow, Photosynthesis, Harvesting light energy, Light driven electron flow.
BOOKS:

MCH-208: GREEN CHEMISTRY 4 Credits

Introduction: Principles of green chemistry – prevention of waste, atom economy, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for energy efficiency, reduce derivatives, renewable feedstock, catalysis, design for degradation, real time analysis for pollution prevention, and inherently safer chemistry for accident prevention.

Green synthesis: clean routes, supercritical solvents, ionic liquids, green catalyst, auto-exhaust catalyst and clean technology.

BOOKS:
1. Real World Cases in Green Chemistry, ACS, M.C. Cann & M.E. Connelly.

MCH-209: PERICYCLIC REACTION, PHOTOCHEMISTRY & REAGENTS 4 Credits

UNIT-I:

UNIT-II:
(a) First order Photochemical processes Light absorption, Fluorescence and Phosphorescence.
(b) Photo reactions: Dissociation, Reduction, Isomerisation, Cycloaddition, Paterno-Buchi reaction, Norrish type I and II reactions, Di-pi-methane reaction, Photochemistry of arenes.

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), Dichloro dicyno benzoquinone (DDQ).

BOOKS:


MCH-210: NANO SCIENCE AND NANOTECHNOLOGY 4 Credits

Introduction: Introduction to Nanoscience; History and Scope of Nanoscience; A Different Kind of Small; Interdisciplinary Sciences behind Nanotechnology and Nanoscience. Carbon Nanotubes, Nanowires Quantum Dots, Nanocrystals, Nanoclusters and other nanostructures


Properties of Nanostructured materials and Measurement Techniques:
- b) Optical Properties: UV-Visible spectroscopy, Raman spectroscopy, IR spectroscopy, Scanning tunneling spectroscopy
- c) Electrical and Thermo-electrical Properties: I-V characterization, C-V characterization
- e) Mechanical and Thermal Properties: Elastic properties, Rheology.
- f) Magnetic Properties: ESR, NMR, Superconducting properties
- g) Chemical Properties: Derivatization of carbon nanotubes and associated characterization methods.
- h) Biomedical: Interaction of Carbon Nanotubes with DNA, Drug delivery, Optical tweezers.

Nanotechnology in Physics, Chemistry, Biology and Engineering: Applications to Nano electromechanical systems (NEMS), Nano-optoelectronic materials and devices, Medical and pharmacology applications, Nanomaterial Thin-films, Optical Limiting properties, Nanoscale devices – Transistors, FETs, quantum dots lasers and others.

BOOKS:
1) Introduction to Nanotechnology by Poole C. P., and Owens F. J., Wiley – India (2006)
2) Nanotechnology: A Gentle Introduction to the Next Big Idea, by Mark A. Ratner
6) Physical Properties of Carbon Nanotubes, by Riichiro Saito, Gene Dresslhaus, and M. S. Dresselhaus, Imperial College Press (London), ISBN 1-86094-093-5,

MCH-211: CHEMISTRY OF MATERIALS  4 Credits

UNIT-I: GLASSES, CERAMICS, COMPOSITES, NANOMATERIALS AND IONIC CONDUCTORS

(b) Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors, phase transition and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

UNIT-II: ORGANIC SOLIDS, FULLERENES, MOLECULAR DEVICES

UNIT-III: THIN FILMS, LANGMUIR – BLODGETT FILMS AND POLYMERIC MATERIALS
(a) Preparation techniques; evaporation/sputtering, chemical processes, MOCVD, sol-gel etc. Langmuir – Blodgett (LB) film, growth techniques, photolithography, properties and application of thin and LB films.
(b) Molecular shape, structure and configuration, crystallinity, stress-strain behaviour, polymer types and their applications, conducting and ferro-electric polymers.
BOOKS:
1. Solid state physics, N. W. Ashcroft and N. D. Mermin, Saunders college
3. Principles of solid state, H. V. Keer, Wiley Eastern
5. Thermotropic liquid crystals, Ed., G. W. Gray, Jhon Wiley
6. Handbook of liquid crystals, Kelker and Hatz, Chemie Verlag

MCH-212: MATERIAL SCIENCE 4 Credits

UNIT – I

UNIT – II
1. Super conductors: Zero resistivity, critical magnetic field and critical current density, Type I and II super conductors, Applications of superconductors.
2. Dielectric materials: Microscopic displacement of atoms and molecules in an external dc electric field, Polarization and dielectric constant, Dielectric susceptibility, Temperature dependence of dielectric breakdown, Ferro electric materials, Piezoelectrics, Pyroelectrics, Dielectric materials as electric insulators.

UNIT – III
2. Organic Materials: Polymers, Mechanism of polymerization, Addition and condensation polymerization, applications; Plastics – Types: Thermosetting and thermoplastics

UNIT – IV
2. Ceramics: Types, Structure, Mechanical properties, applications
BOOKS:
2. Vijaya MS, Rangarajan G, Materials Science, TMH.
3. Rajendran V, Marikani A, Materials Science, TMH.

MCH-213:  MEDICINAL CHEMISTRY        4 Credits

**Drug Design:** The drug discovery process - conceptual back-ground - Drug receptors - drug target binding forces – History and development of QSAR – effect of physical properties of the drug on its action (Ferguson and related theories)- concept of lead structure & pharmacophore – concept of isosterism and bioisosterism- three dimensional structure - aided drug design (use of PC Spartan / Hyperchem lite / PC Spartan plus software packages, to get hands on experience).

**Pharmacokinetics & Pharmacodynamics:** Introduction of drug absorption, bioavailability (factors effecting and dosage determination) and metabolism -Phase I & PhaseII .

A **study of antibiotics:** Chemistry and pharmacology of streptomycin, Structure and Pharmacology of tetracyclines, gramicidin, a survey of anticancer antibiotics

**Dietary factors:** Study of water-soluble vitamins Chemistry and biological functions of thiamine, riboflavin, pyridoxine, pantothenic acid and folic acid.

**Drugs from medicinal plants:** A study of active ingredients of some well-established Indian medicinal plants; A survey of Chinese medicinal plants.

**PREScribed BOOKs:**

**REFERENCE BOOKS:**
3) Kirk Othmer's Encyclopaedia of Chemical Technology 3rd edition, Wiley Interscience Publication. 1978 - 84
MCH-214: NATURAL PRODUCTS AND SPECTROSCOPY-II  4 Credits

UNIT-I:
(a) Alkaloids: Morphine (Structure elucidation, Synthesis, Molecular rearrangement and Stereochemistry)
(b) Steroid: Cholesterol (Structure elucidation, Synthesis).
(c) Terpenes: Abietic acid (Structure elucidation, Synthesis).

UNIT-II:
NMR: 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-III:
(a) Mass spectrometry: Introduction, Mass spectrum, Determination of molecular formulae, Parent peak, Base peak, Use of molecular fragmentation, Mass spectra of some classes of compounds (hydrocarbons, alcohols, phenols, ketones, aldehydes, acids and esters).
(b) Problems involving UV, IR, NMR and Mass spectroscopy.

BOOKS:
1. Chemistry of Natural products : Sharma and Agrawal,
2. Organic Chemistry II : I.L. Finar

MCH-215: SOLID STATE CHEMISTRY AND NANO MATERIALS  4 Credits

Preparative methods: Solid state reactions general principles, experimental procedure, coprecipitation as a precursor to solid state reactions, kinetics of solid state reactions, crystallization of solutions, melts, glasses and gels, vapour phase transport methods, ion exchange reactions, intercalation / deintercalation reactions, electro chemical reduction methods and thin film preparation.growth of single crystals.

X-Ray Diffraction: X-rays and their generation-an optical grating and diffraction of light, crystals and diffraction of x-rays, X-ray diffraction experiment, the powder method-principles and uses, single crystal methods-principle and uses. High temperature X-ray diffraction, electron diffraction and neutron diffraction.

Electronic properties and band theory: Metals, insulators and semiconductors, colour in inorganic solids.other electrical properties-hall effect, dielectric materials, ferro-pyro-piezo electricity and its applications.

Magnetic properties: Dia, para, ferro, ferri, and antiferro magnetic types-selected magnetic materials such as spinels, garnets and perovskites.
**Superconductivity:** Theory, discovery and recent high Tc materials Organic solids state chemistry—electrically conducting solids, organic charge transfer complex, organic metals, new super conductors.


**BOOKs:**
2) Introduction to Nanotechnology by Poole and Owens, Wiley, 2003

**MCH-216: SUPRAMOLECULAR CHEMISTRY**

4 Credits

**Host - Guest complexation chemistry:** Basic concepts, molecular recognition, complex formation and host design – Macrocycles, clefts and open chain host structures, thermodynamics of multi-site hostguest complexation.

**Non-covalent interactions and organic host guest complexes:** Ionic, hydrogen bonding, cation – pi electron interactions, Van der waals, stacking and charge transfer interactions and their quantification.

**Ionophores for cations and anions:** chelate, macrocyclic and cryptate effects, complexation selectivity, thermodynamics (enthalpy, entropy and heat capacity changes), macrocycles with secondary binding sites, effect of solvent.

**Crown ethers:** synthesis of all oxygen, all nitrogen, all sulphur & oxygen - nitrogen bridged systems, use of crown ethers in Organic Synthesis, binaphthyl crown ethers (CPK models) in racemic resolution.

**Cyclodextrins:** Ester hydrolysis, model of carbonic anhydrase (Tabushi’s model) - Micelles, their use in organic Synthesis, Breslow’s remote functionalization using substituted benzophenones.

**Bio - organic chemistry of the Phosphates:** Biological role of phosphate macromolecules – General properties, experimental evidences for DNA double helix-chemical synthesis of polynucleotides (trinucleotide)- role of other nucleotide phosphates (NADP, FAD, CAMP & CGMP)

**Selected applications:** Synthetic classification of organic electron transfer reactions - Marcus Theory – Photoinduced intramolecular electron transfer systems - introduction to molecular switches – optical devices, electrochemical devices.

**Nanotechnology:** Introduction, nanobiotechnology - applications in medicine.
BOOKS

REFERENCE BOOKS:

MCH-217: BIOCATALYSIS FOR INDUSTRY, MEDICINE AND ENVIRONMENT 4 Credits

Bio transformation, Biocatalyst and Chemical Industry:
Basic organic reaction mechanism, common prejudices against enzymes, advantages and disadvantages of biocatalysys, isolated enzyme versus whole cell systems, Enzymatic and Microbial


Immobilized Enzymes and Immobilized Microorganisms, Principal Immobilization techniques, Lipase powders, Enzymes Covalently Bonded on Neutral Polymers, Cross-Linked Enzyme Crystals (CLEC), Treatments of Whole Cells Medium Engineering Cofactor Regeneration Techniques

Microbial Kinetics
Reaction theory and kinetics, Cell growth and kinetics, Yield and maintenance, coefficient concepts, Determination of microbial kinetics from batch data, Substrate utilization and product formation kinetics.

Fermentor Operation
Batch, fed-batch and chemostat operation of bioreactors, Evaluation of kinetic and yield parameters in chemostat culture, Bioreactor configurations, Fermentor operation – initiation, operation and harvest of batches

Application of Biotechnology to Chemical Production, Single-step Reactions of Commercial Importance, Multi-step Reactions of Commercial Importance
Biological Routes to Optically Active Epoxides, The Production of Optically Pure Natural and Unnatural Amino Acids, hydro-xylation of steroids at unactivated carbon centers, Case Study.
**Bioremediation and Biological Method for Pollution Control:**

**Environmental remediation:** Bioremediation and biodegradation - molecular biological approaches to sustainable development. Oil bioremediation, radio tracer methodology, anaerobic and aerobic degradation, site characterization, treatability assessment, remediation technology selection, and design of in situ remediation techniques, Case Study.

**Environmental enhancement:** Positive intervention: molecular biological approaches to increasing biochemical tolerance (crop protection, fertilisers, biogeochemical processes); Clean technologies: biotechnological alternatives to present energy sources and commodity production; Waste control: regulation, reduction, recycling, Case Study.

**Medicinal Biotransformations: Drug Metabolism:**
Overview of biotransformation and excretion routes for xenobiotics in mammals; methods for study; metabolic detoxification and activation. Phase 1 and phase 2 biotransformation; characteristics. Microbial models for mammalian metabolism. Downstream processing, Production of antibiotics, semi-synthetic analogues.

**BOOKS:**
2) Biotreatment of Industrial Effluents, Doble Mukesh and Anil Kumar, Elsevier, USA, 2005.
7) Medicinal Chemistry by Foye, 1990.

**REFERENCE BOOKS:**

**MCH-218: BIO-INORGANIC CHEMISTRY 4 Credits**

**New perspectives and biological roles of essential trace elements.**

**Oxygen carriers:** Transport and storage of dioxygen - reactions of dioxygen- structure and functioning of hemoglobin and myoglobin – Hemerythrins – Hemocyanin - Model compounds for oxygen carriers (Vaska’s iridium complex, cobalt - DMG complex).
Biological nitrogen fixation: Nitrogen fixing organisms - structure and function of nitrogenase enzyme - Chemistry of nitrification - Fixation via nitride formation - Dinitrogen complexes as biological models.


Alkali metal transport in Biological systems: Introduction - Coordination chemistry of alkali metal ions-lon transport - Modes of passage - Sodium dependent transport.

Metal ions toxicity and Chelation therapy: Toxicity of metal ions particularly heavy metal ions - Chelating agents-chelation therapy - Therapeutic uses of metals, ligands and complexes with special reference to anti-cancer activity.

Biomineralisation: Nucleation and crystal growth, calcium phosphate, calcium carbonate, amorphous silica, iron biominerals, strontium and barium sulphates.

BOOKS:

REFERENCE BOOK:

MCH-219: FERROUS-NONFERROUS METALLURGY  4 Credits

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(Head of the Department)
Chemistry

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