

**VEER SURENDRA SAI UNIVERSITY OF  
TECHNOLOGY  
(VSSUT)**



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

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

**SEMESTER SYLLABUS**

<b>COURSE NO</b>	<b>COURSE TITLE</b>	<b>CREDITS</b>
<b>1<sup>st</sup> SEMESTER</b>		
MCH-101	GROUP THEORY & QUANTUM CHEMISTRY	<b>4</b>
MCH-102	COORDINATION CHEMISTRY	<b>4</b>
MCH-103	STRUCTURE AND REACTIVITY	<b>4</b>
MCH-104	STEREOCHEMISTRY	<b>4</b>
MCH-105	THERMODYNAMICS & ELECTRO CHEMISTRY	<b>4</b>
MCH-191	INORGANIC GENERAL PRACTICAL	<b>2</b>
MCH-192	ORGANIC GENERAL PRACTICAL	<b>2</b>
<b>TOTAL</b>		<b>24</b>
<b>2<sup>nd</sup> SEMESTER</b>		
MCH-106	ANALYTICAL CHEMISTRY	<b>4</b>
MCH-107	SPECTROSCOPY-I	<b>4</b>
MCH-108	ORGANIC REACTION MECHANISM	<b>4</b>
MCH-109	POLYMER CHEMISTRY	<b>4</b>
MCH-110	SURFACE CHEMISTRY & NUCLEAR CHEMISTRY	<b>4</b>
MCH-193	PHYSICAL GENERAL PRACTICAL	<b>2</b>
MCH-194	ANALYTICAL CHEMISTRY PRACTICAL	<b>2</b>
<b>TOTAL</b>		<b>24</b>
<b>3<sup>rd</sup> SEMESTER</b>		
	2 Elective Courses (2x4) should be selected	<b>8</b>
MCH-201	MATERIAL AND ENERGY BALANCE	<b>4</b>
MCH-202	ENVIRONMENTAL CHEMISTRY	<b>4</b>
MCH-203	INDUSTRIAL PROCESSES	<b>4</b>
MCH-291	INDUSTRIAL PRACTICAL	<b>2</b>
MCH-292	ENVIRONMENTAL CHEM PRACTICAL	<b>2</b>
<b>TOTAL</b>		<b>24</b>
<b>4<sup>th</sup> SEMESTER</b>		
	1 Elective Courses should be selected	<b>4</b>
MCH-293	Review/ Industrial project/ Research project	<b>10</b>
MCH-294	Seminar	<b>4</b>
MCH-204	COMPUTER APPLICATION IN CHEMISTRY	<b>2</b>
MCH-295	PRACTICAL ON COMPUTER IN CHEMISTRY	<b>2</b>
MCH-296	INDUSTRIAL TRAINING REPORT	<b>2</b>
<b>TOTAL</b>		<b>24</b>

<b>ELECTIVE COURSES FOR 3<sup>rd</sup> AND 4<sup>th</sup> SEMESTERS</b>		
<b>COURSE NO</b>	<b>COURSE TITLE</b>	<b>CREDITS</b>
<b>3<sup>rd</sup> SEMESTER</b>		
MCH-205	INSTRUMENTAL METHODS OF ANALYSIS	<b>4</b>
MCH-206	INDUSTRIAL POLLUTION AND ITS MANAGEMENT	<b>4</b>
MCH-207	BIOCHEMISTRY	<b>4</b>
MCH-208	GREEN CHEMISTRY	<b>4</b>
MCH-209	PERICYCLIC REACTION, PHOTOCHEMISTRY & REAGENTS	<b>4</b>
MCH-210	NANO SCIENCE AND NANOTECHNOLOGY	<b>4</b>
MCH-211	CHEMISTRY OF MATERIALS	<b>4</b>
<b>4<sup>th</sup> SEMESTER</b>		
MCH-212	MATERIAL SCIENCE	<b>4</b>
MCH-213	MEDICINAL CHEMISTRY	<b>4</b>
MCH-214	NATURAL PRODUCTS & SPECTROSCOPY-II	<b>4</b>
MCH-215	SOLID STATE CHEMISTRY AND NANO MATERIALS	<b>4</b>
MCH-216	SUPRAMOLECULAR CHEMISTRY	<b>4</b>
MCH-217	BIOCATALYSIS FOR INDUSTRY, MEDICINE AND ENVIRONMENT	<b>4</b>
MCH-218	BIOINORGANIC CHEMISTRY	<b>4</b>
MCH-219	FERROUS-NONFERROUS METALLURGY	<b>4</b>

## 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,  $C_n$ ,  $C_{nv}$ ,  $C_{nh}$ ,  $S_n$ ,  $D_n$ ,  $D_{nd}$ ,  $D_{nh}$ ,  $T_d$ ,  $O_h$ ,  $D_{\infty h}$ ,  $C_{\infty v}$  and  $D_{\infty h}$ , properties of point groups, group theoretical representations, Orthogonality theorem, construction of character tables for  $C_{2v}$ ,  $C_{3v}$ , T (cubic),  $C_4$  (cyclic) and  $D_{\infty h}$  groups, projection operator and direct product.

##### UNIT-II: WAVE MECHANICS OF SOME SYSTEMS

Application of Schrodinger 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 Russel-Saunders's term for  $P^2$ ,  $d^2$  and  $pd$  configuration.

##### UNIT-III: APPROXIMATION METHOD

The variation theorem and its application to Hydrogen atom in derivation of its ground state energy, the secular equations, the LCAO approximation (molecular orbital theory) and its 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 over all 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:

Introduction to stability constants - Factors affecting stability constants - Kinetic and thermodynamic stability - Irwing-William series - concept of Hard and Soft acids and bases - Methods of determining stability constants (spectrophotometric, conductometric and pH-metric methods).

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:**

- 1) Inorganic chemistry by J.E.Huheey, E.A.Keiter and R.L.Keiter, Harper collins, 4th Ed., 1993 .
- 2) Advanced Inorganic Chemistry by F.A.Cotton and G.W.Wilkinson, John-Wiley 5th Ed., 1988.
- 3) Mechanisms of Inorganic Reactions by F.Basolo and R.G.Pearson, Wiley Eastern, 2nd Ed., 1977.
- 4) Coordination Chemistry by F.Basolo and R.Johnson, W. A. Benzamin Inc., 1964.
- 5) Coordination Chemistry by D.Banerjea, Tata-McGraw-Hill 1993.
- 6) Complexes and First Row Transition Elements by D.Nichols, Macmillan 1974.
- 7) Molecular Magnetism by O.Kahn, Wiley VCH,1993

**REFERENCE BOOKS:**

- 1) Photochemistry of Coordination Compounds by V. Balzani & V. Carasitti, Academic Press, New York 1970.
- 2) Concepts and Models of Inorganic Chemistry by B. Douglas, D.H. McDaniel & J.J. Alexander, 2nd Ed., John Wiley, New York 1983.
- 3) Transition Metal Chemistry by M. Gerloch & E.C. Constable, VCH Publications New York, 1994.
- 4) Kinetics and Mechanisms of Reactions of Transition Metal Complexes by R.G. Wilkins, 2<sup>nd</sup> Ed., VCH publications, 1991.
- 5) Inorganic Reaction Mechanisms by Martin L. Tobe and John Burgess, Longman, 1999.
- 6) Reaction mechanisms of Inorganic and Organometallic systems, 2<sup>nd</sup> Ed; by Robert B. Jordan, Oxford University Press, Oxford, 1991.
- 7) Inorganic Chemistry by Gary Wulfsberg, USB, California, 2000.

**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)
3. Mechanism and theory in organic chemistry : T. H. Lowry and K S Richardson(Harper Row Publishers, New York)
4. Organic Chemistry : Morrison and Boyd.

**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 biphenyls and allenes, Concept of Prostereoisomerism and Assymmetric synthesis (including enzymatic and catalytic nexus), Conformation of a few acyclic molecules (alkanes, haloalkanes), Conformation of cyclic systems having one and two sp<sup>2</sup> carbon atoms.

## UNIT-II:

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, 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 dichroism, 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:**

1. Stereochemistry of organic compounds : D. Nashipuri.
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, Isoelectric points.

UNIT-V: CHEMICAL KINETICS

Theories of reaction rates, Collision theory, Transition state theory of uni and bimolecular reactions, Lindemann mechanism. Arrhenius and activated complex, Reaction between ions, Salt effect, Steady-State Kinetics, Kinetic and Thermodynamic concept of Reactions, Dynamic chain ( $H_2 + Br_2$  reaction, pyrolysis of  $CH_3CHO$ , 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:**

1. Text Book of Physical Chemistry Vol-1-4 : K.L. Kapoor
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. Chemical Thermodynamics : R.P. Rastogi & S.S. Mishra
7. Thermodynamics for Chemists : S. Glasstone
8. Thermodynamics for Irreversible Processes : S. Hasse
9. Thermodynamics for Irreversible Processes : L Prigogine
10. Principle of Biochemistry : A.L. Lehninger



11. Electrochemistry	: S. Glasstone
12. Modern Electrochemistry Volume-I	: Bookris & Reddy
13. Chemical Kinetics	: Frost & Pearson
14. Chemical Kinetics	: J.L. Agrawal
15. Chemical Kinetics	: K.J. Laidler

**REFERENCE BOOKS:**

- 1) Electrochemistry theoretical foundation - J.Goodieman John wiley sons 1987.
- 2) Spectro electrochemistry - Theory and Practice R.J.Gale, Plenum Press New York, 1988.
- 3) Principles of colloids and surface chemistry, 2nd edition, P.C. Hiemenz. Marcel Dekker, INC. 1986.
- 4) Physical chemistry of surfaces, 6th Ed. A.W. Adamson and A.P. Gast, John Wiley & sons 1997.
- 5) Introduction to Thermodynamics of Irreversible Processes by I. Prigogine, 3rd Ed. Interscience Publishers, 1967.

**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:**

- 1) Principles of Instrumental Analysis, by D.A.Skoog, F.J. Holler and T.A. Nieman, 5th Ed., Saunders College publishing 1998.
- 2) Laboratory Techniques in Electro Analytical Chemistry by P.T.Kissinger and W.R. Heineman, Marcel Dekker Inc. New York 1984.
- 3) Kinetic Aspects of Analytical Chemistry by H.A.Mottola, John Wiley and Sons, 1988.
- 4) Radio Analytical Chemistry Vol.I & II by J.Tolgyessy and M.Krys. Ellis Horwood Ltd, 1989.
- 5) Fundamentals of Analytical Chemistry by D.A.Skoog, D.M.West and F.J.Holler. Saunders College Publication, New York - 5th Ed., 1988
- 6) Analytical Electrochemistry by Joseph Wang, Wiley VCH, 2006

**REFERENCE BOOKS:**

- 1) Supercritical Fluid Chromatography by R.M.Smith, The Royal Society of Chemistry 1988.
- 2) Perspectives in Modern Chemical Spectroscopy by D.L.Andrews Springer verlag, 1990
- 3) Analytical Chemistry G.D.Christian, 5th Ed. John - Wiley & Sons 1994.
- 4) Qualitative analysis by R.A.Day Jr., A.L. Underwood 5th Ed., Prentice Hall of India, 1988.
- 5) Vogel's textbook of Quantitative Chemical Analysis (revised copy), 5th Ed., ELBS, 1994.

**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:**

1. Text Book of Physical Chemistry Vol-1-4 : K.L. Kapoor
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
8. Spectroscopy Vol. I & II : Walker & Straw
9. Fundamentals of Molecular Spectroscopy : C.N. Banwell
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 carbocations, phenonium ions, norbornyl system, common carbocation rearrangements, application of NMR spectroscopy in the detection of carbocations. 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, Vilsmeier - Haack reaction, Pechmann reaction.

UNIT-III:

- (a) Aromatic Nucleophilic Substitution mechanism: Introduction, to different mechanisms, Aromatic nucleophilic substitutions ( $S_NAr$ ,  $S_N1$  aryl), Effect of substrates, leaving groups, and nucleophile, Reactions: Nucleophilic displacement in aryl-diazonium salts by different nucleophiles, Chichibabin reaction.
- (b) Free radical Substitution: Reaction at  $sp^2$  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,  $LiAlH_4$  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:

Elimination mechanism:  $E_1$ ,  $E_2$ ,  $E_1CB$  and  $E_2CB$  mechanisms, Orientation, Effect of substrate, base, leaving group and medium, Orientation of double bond, Saytzeff and Hoffman rules, Pyrolytic elimination reaction, Oxidative elimination (oxidation of alcohol by chromium, Moffatt oxidation). Reactions: Cleavage of quaternary ammonium hydroxides, Chugaev reaction, Shapiro reaction.

UNIT-VI:

REARRANGEMENTS

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

Wagner-Meerwein, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofmann, Schmidt, Lossen, Curtius, Baeyer-Villiger, Shapiro reaction, Von-Richter, Sommelet-Hauser rearrangement.

**BOOKS:**

1. Advanced organic chemistry: Reaction mechanism and structure : Jerry March (Wiley Eastern Limited)
2. Organic reaction mechanism: Kalsi,
3. Physical Basis of Organic Chemistry: N. Isaac, (Wiley Eastern Limited)

**Step Polymerisation:**

Mechanism of step polymerisation - kinetics of step polymerisation - molecular weight control in linear polymerisation - molecular weight distribution in linear polymerisation polyfunctional step reaction polymerisation - Newer types of 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 utilizations.

**Mechanical behaviour of polymers:**

An energy balance for deformation and fracture - deformation and fracture in polymers - crack growth, cyclic deformations - molecular aspects of fracture and healing in polymers - behaviour of adhesives. Conducting polymers: General characteristics with examples. Polymer molecular weight - different types - their determination.

**BOOKS:**

- 1) Text Book of Polymer Science by F.W.Billmeyer, Jr. 3rd Ed., John Wiley & Sons 1984.
- 2) Introduction to Polymers by R.J.Young and P.A.Lovell, 2nd Ed., Chapman & Hall 1991.
- 3) Contemporary Polymer Chemistry by H R Allcock and F.W.Lampe, Prentice Hall, New Jersey, Second Ed 1990.
- 4) Principles of Polymerisation by G.Odian 3rd Ed., John Wiley & Sons., 1991.
- 5) Introduction to Physical Polymer Science, 2nd Ed., L. H. Sparling, John Wiley & Sons, 1993.

**REFERENCE BOOKS:**

- 1) Polymer Chemistry by M.P.Stevens, 2nd Ed ,Oxford University Press,. 1990.
- 2) Polymer Chemistry by R.B.Seymour and C.E.Carraher Jr., 3rd Ed., Marcel Dekker Inc, 1992.

**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**

Surface tension, Capillary action, 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, Brief concepts on micelle, reversed micelle and microemulsions.

**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:**

1. Text Book of Physical Chemistry Vol-1-4 : K.L. Kapoor
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. Introductory Quantum Chemistry : A.K. Chandra
7. Molecular Quantum Mechanics : P.W. Atkins
8. Notes on Molecular Orbital Calculations : J.D. Roberts
9. Polymer Science : V.R. Gowariker,  
N.V.Viswanathan  
& J. Sreedhar

*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:**

1. G. Friendlander, J.W. Kennedy & J.M. Miller Nuclear and Radiochemistry, Wiley Interscience, New York.
2. B.G. Harvey, Introduction to Nuclear Physics & Chemistry, Prentice - Hall, Englewood Cliffs (N.J)/ Prentice-Hall, India, EEE Edn.
3. R.T. Overman, Basic concept of Nuclear Chemistry, Chapman & Hall.
4. A. N. Nesmeyanov, Radiochemistry, MIR Publication, Moscow.
5. J.W.T. Spinks & R.J. Woods, An Introduction to Radiation Chemistry, Wiley, New York.
6. H. J. Arnika, Essentials of Nuclear Chemistry, Wiley Eastern Ltd., 2nd Edition.

**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+CH<sub>3</sub>COOH with NaOH
4. Determination of solubility product of BaSO<sub>4</sub>.
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<sup>+2</sup>.
11. To study of an equilibrium  $KI + I_2 = KI_3$ .
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 2Credits**

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**

- (a) Material Balances Without Chemical Reactions: Process Flow-Sheet, Material Balances, Recycling Operations, Material Balances of Unsteady State Operations.
- (b) Material Balances Involving Chemical Reactions, Definition of Terms, Electrochemical Reactions, Recycling, Parallel and Bypassing Operations, Metallurgical Applications

**UNIT-II: ENERGY BALANCES**

Energy and Thermo-Chemistry, Energy Balances, Heat Capacity, Heat Capacity of Gases at Constant Pressure, Sensible Heat Changes in Liquids, Heat Capacity of Gaseous Mixtures, Latent Heats, Enthalpy Changes During Phase Transfers Accompanied by Sensible Heat Changes, Enthalpy Changes Accompanying Chemical Reactions, Effect of Temperature on Heat of Formation, Heat of Reaction, Adiabatic Reactions, Effect of Pressure on Heat of Reaction, Thermochemistry of Mixing



Process, Dissolution of Solids, Liquid-Liquid Mixtures, Heat of Solution by Partial Molal Quantities.

### UNIT-III: STOICHIOMETRY AND UNIT OPERATIONS

Distillation, Absorption and Stripping, Extraction and Leaching, Crystallisation, Psychrometry, Drying, Evaporation, Less Conventional Operation.

#### BOOKS:

1. Advance Inorganic Chemistry: F.A.Cotton , G.Wilkinson & C. Murillo (6<sup>th</sup> edition)
2. Inorganic Chemistry : J.E.Helay, Harper and Row
3. Comprehensive Coordination Chemistry: Eds.Wilkinson,Gillarsand (Pergamon Press)
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 radionuclides - Biochemical oxygen demand-Chemical oxygen demand, Eutrophication, Biodegradation of pollutants.

**Water treatment:** Hardness of water and its removal - removal of solids and other toxic materials - Treatment of water for drinking - Electrodialysis, ion exchange, reverse osmosis, desalination processes, removal of iron, manganese, phosphorous, calcium and nitrogen and Treatment of water for industrial purposes - sedimentation, coagulation, flocculation, filtration, adsorption, disinfection of water - Sewage treatment (physical and chemical methods) - Health effects of drinking water treatment technologies – Impact of detergents, pesticides and other additives on sewage treatment.

**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.

**Hazardous Wastes:** Nature and sources of hazardous wastes - classification, characteristics & constituents - transport and effects - hazardous wastes in Geosphere, Hydrosphere, Biosphere and Atmosphere - reduction, treatment by physical and chemical methods - Thermal treatment methods - Biodegradation of wastes - Disposal of hazardous wastes. Waste management and Industrial byproducts- Natural hazards and management-control of subsurface migration of Hazardous Waste.

**Values in Environment:** The philosophy and Technology of living in tune with with nature and its asseete. Nature-A silent teacher Ecology-The Indian Approach

**BOOKS:**

- 1) Environmental Chemistry by Stanley E.Manahan, 5th Ed., Lewis , 1991.
- 2) Oil in Fresh Water - Ed., Vander Meulen and Hruday, Pergamon , 1987.
- 3) Chemical Contamination in The Human Environment by Lippmann and Schlesinger, OUP,Oxford, 1979.
- 4) Environmental Pollution by H.M.Dix., Wiley, 1981.
- 5) Environmental Chemistry by A.K.De., 2nd Ed., Wiley Eastern 1989.
- 6) Water Treatment - Principles and Design by J.M.Montgomery., Wiley, 1985.
- 7) Pollution: Causes, Effects and Control by R.M. Harrison, 3rd Ed., Royal Society of Chemistry, London,1996.

**REFERENCE BOOKS:**

- 1) Atmospheric Chemistry by B.J.Finlayson – Pits and N.N.Pitts Jr., Wiley, 1986.
- 2) Hazardous and Industrial Wastes – Ed., .M.M.Varma, HMCRI, 1988.
- 3) Water Treatment - Principles and Design by J.M.Montgomery., Wiley, 1985.

**MCH-203: INDUSTRIAL PROCESSES**

**4 Credits**

**UNIT-I:**

Petroleum and coal based chemicals: Composition of petroleum, cracking processes, Commercial production of ethylene, acetylene, polymerization mechanisms, Addition, condensation, step growth, chain growth, method of polymerization, Distillation of coal.

**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:**

1. Outlines of Chemical Technology. By M. Gopala Rao and Marshall Sittig, Affiliated East-West Press Pvt. Ltd.
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 chlorine in bleaching powder.
5. Determination of flash point of a lubricating oil.
6. Determination of viscosity of a lubricating oil.
7. Determination of calorific value, carbon residue, volatile matter of a sample of coal.

**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<sup>++</sup>: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
5. Computer Aids to Chemistry: Ed. G. Vernin & M. Chanon

**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 3<sup>rd</sup> AND 4<sup>th</sup> 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<sub>x</sub>, NO<sub>x</sub>, CO<sub>2</sub>, 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:**

1. Environmental Chemistry, S. K. Banerji, Prentice Hall, India, New Delhi 1997
2. Environmental Chemistry, A. K. Dey
3. A text book of Environmental chemistry and pollution control, S S Dara, S. Chand Company, Delhi, 1997.
4. Industrial Chemistry, B. K. Sharma, Goel Publishing house, Meerut, 1997.

**MCH-207: BIOCHEMISTRY**

**4 Credits**

**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: Over view, 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,  $\beta$ -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:**

1. Principles of Biochemistry: A. L. Lehninger, D. L. Nelson and M. Cox (CBS Publishers and Distributors)
2. Biochemistry: L. Stryer (W. H. Freeman Company, New York, 1988)

**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.
2. Green Chemistry: Designing Chemistry for Environment, ACS, P.T. Anastas and T.C. Williamson.
3. Green separation processes, methods and application, Fonso, National Scientific Book Agency, Delhi-110053.

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

## UNIT-I:

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 Correlation diagrams. FMO and aromatic transition state concept. Electrocyclic reactions - Con-rotatory and dis-rotatory motions,  $4n$ ,  $4n+2$  and allyl systems. Cycloaddition reactions - Supra- and Antara-facial additions,  $4n$  and  $4n+2$  systems, 2+2 additions of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements - Supra and Antara-facial shifts of H, Sigmatropic shift of carbon moieties, 3,3- and 5,5-sigmatropic rearrangements, Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

## 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 dicyano benzoquinone (DDQ).

**BOOKS:**

1. Conversion of Orbital symmetry : R. B. Woodward and Hoffman
2. Organic reactions and orbital symmetry: T. L. Gilchrist and R. C. Storr
3. Mechanism and theory in organic chemistry: T. H. Lowry and K. S. Richardson.
4. Basic Principles of Organic Chemistry: J. D. Roberts and M. C. Casserio

**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

**Synthesis Methods and Strategies:** Measuring and Imaging Tools for Nanostructures; Preparation, Synthesis and Fabrication of Nanostructures - Laser Vaporization, Electric-arc, CVD, Laser Pyrolysis, Hydrothermal, Gas Phase Synthesis and Sol-Gel Processing, Self-Assembly.

**Properties of Nanostructured materials and Measurement Techniques:**

- a) Structural Properties: Electron Microscopy and Diffraction, X-ray Diffraction, Atomic Force Microscopy, Energy dispersive Analysis, Scanning tunneling microscopy / spectroscopy
- 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



- 3) Daniel Ratner, Mark Ratner, Prentice Hall PTR; 1st edition (2002), ISBN: 0446679569.
- 4) Nano: The Essentials, by Pradeep T., Tata McGraw Hill (2007).
- 5) Understanding Nanotechnology, Scientific American, Warner Books (2002), ISBN: 0131014005.
- 6) Physical Properties of Carbon Nanotubes, by Riichiro Saito, Gene Dresselhaus, and M. S. Dresselhaus, Imperial College Press (London), ISBN 1-86094-093-5,
- 7) Nanostructured Forms of Carbon: An Overview, by A. M. Rao and M. S. Dresselhaus, in Nanostructured Carbon for Advanced Applications, Eds. G. Benedek, P. Milani, V. G. Ralchenko, Kluwer Academic Publishers, (2001)
- 8) Nanostructure Science and Technology: A Worldwide Study, Eds. by R.W. Siegel, E. Hu, M.C. Roco, National Science and Technology Council (NSTC), U.S.A, Report 1999.

**MCH-211: CHEMISTRY OF MATERIALS**

**4 Credits**

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

- (a) Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Refractories, characterizations, properties and applications. Macroscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, special properties, applications.
- (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**

Conducting organics, organic superconductors, magnetism in organic materials. Fullerenes – doped, fullerenes as superconductors. Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches-sensors. Nonlinear optical materials: nonlinear optical effects, second and third order – molecular hyperpolarisability and second order electric susceptibility – materials for second and third harmonic generation.

**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, cryatallinity, 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
2. Material science and engineering, An introduction, W. D. Callister, Wiley
3. Principles of solid state, H. V. Keer, Wiley Eastern
4. Materials science, J. C. Anderson, K. D. Leaver, J. M. Alexander and R. D. Rawlings, ELBS
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**

1. Classification of Engineering materials: Engineering properties of materials, Internal structure, Properties.
2. Electron theory of solids: Free electron theory of metals, Electrical conductivity, Thermal conductivity, Quantum theory of free electrons, Band theory o solids, Conductivity of metals.
3. Conductors, Insulators, Semiconductors, Intrinsic and extrinsic semiconductors, Band theory of conductors, Hall effect.

**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.
3. Magnetic Properties: Dia, para and ferro magnetic materials, Theory of magnetism, Ferri magnetic materials or ferrites, Comparison of magnetic behaviour and magnetic parameters of Dia, para and ferro magnetic materials.

**UNIT – III**

1. Optical properties of Materials: Scattering, Refraction, Theory of Refraction and absorption, Atomic theory of optical properties, Lasers, Optical fibers-Principle, structure, application of optical fibers.
2. Organic Materials: Polymers, Mechanism of polymerization, Addition and condensation polymerization, applications; Plastics – Types: Thermosetting and thermoplastics

**UNIT – IV**

1. Composite materials, Agglomerated materials, Cermets, Reinforced materials, Reinforced concrete, Glass fibre reinforced plastics, Carbon fibre reinforced plastics, Whiskers, fibre reinforced plastics, Laminated plastic sheets, Tufnol, Properties of composites.
2. Ceramics: Types, Structure, Mechanical properties, applications
3. Performance of materials in Service: Service performance, failure, design considerations, Corrosion types (Atmospheric, Pitting, Stress corrosion), Control and prevention, protective coating, Performance of metals and ceramics at high temperature.

**BOOKS:**

1. Callister WD, Materials Science and Engineering, John Wiley & Sons.
2. Vijaya MS, Rangarajan G, Materials Science, TMH.
3. Rajendran V, Marikani A, Materials Science, TMH.
4. Van Vlack LH, Elements of Material Science and Engineering, Addison Wesley.

**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:**

- 1) Burger's Medicinal chemistry, Volume I, Ed.- M.E.Wolff, 5th Ed., John Wiley & Sons, 1995.
- 2) Principles of Medicinal Chemistry, Edited by N.O.Foye, Lea and Febiger; Philadelphia, 1976.
- 3) Comprehensive Medicinal Chemistry Vol 4 , Edited by C. Hansch, P.G. Sammes and J. B. Taylor, Quantitative Drug Design, Pergamon Press, 1990.
- 4) Molecular Recognition of Amiloride Analogs: A Molecular Electrostatic Potential Analysis, J. Med. Chem., 35, p 1643, 1992.

**REFERENCE BOOKS:**

- 1) Introductory Medicinal Chemistry by J.B.Taylor and P.D.Kennewell, Ellis Horwood, 1981.
- 2) Modern Drug Research, Vol.12, Paths to better and safer drugs edited by Yvonne Connloy Martin, Eber Hard Kutter, Volkhard Sustel., Marcel Dekker. Inc, 1989.
- 3) Kirk Othmer's Encyclopaedia of Chemical Technology 3rd edition, Wiley Interscience Publication. 1978 - 84
- 4) Ullmann's Encyclopaedia of Industrial Chemistry VCH Publishers, Wurzburg, Federal Republic of Germany, 1987-89.
- 5) Remington's Practice of Pharmacy, 13th Ed., The Mach Publishing Company, Eastern P.A. 1979.

**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,  $^{13}\text{C}$ ,  $^{15}\text{N}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$  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
3. Spectroscopic identification of organic compounds : R. N. Silverstein & G. C. Basselor

**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 T<sub>c</sub> materials Organic solids state chemistry-electrically conducting solids, organic charge transfer complex, organic metals, new super conductors.

**Liquid crystals:** Mesomorphic behaviour, thermotropic liquid crystals, nematic and smectic mesophases. Optical and dielectric properties of liquid crystals. Lyotropic phases and their description of ordering. Carbon Nano tubes- An introduction to synthesis, structure, reactions, carbon molecules, carbon clusters, and applications of carbon nanotubes.

#### **BOOKS:**

- 1) Solid state chemistry and its applications, by A. R. West, W. S. E. Wiley. 2003.
- 2) Introduction to Nanotechnology by Poole and Owens, Wiley, 2003
- 3) Nanochemistry: A Chemical Approach to Nanomaterials. by Geoffrey A Ozin (Author), André C Arsenault (Author) Royal Society of Chemistry, 2005.
- 4) Introduction to solids. L.V. Azaroff, Tata McGraw Hill, 1977.
- 5) Solid state chemistry, L. Smart and E. Moore, Chapman Hall 1992.

#### **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

1. Principles and methods in Supramolecular Chemistry – Hans-Jorg Schneider and Anatoly Yatsimirsky, John Wiley & Sons, LTd., England, 2000.
2. Handbook of Organic Conductive Molecules and Polymers, Ed. By Hari Singh Nalwa, John Wiley & Sons, England, 1977.

## REFERENCE BOOKS:

1. Advances in Physical Organic Chemistry, Vol.18, Academic Press, 1982.
2. Topics in Carboxylic Chemistry, Ed. Douglas Lloyd, Plenum Press, p269, 1969.
3. The Chemistry of Functional Groups, Ed. Saul Patai, Supplement E, Part 1, John Wiley and Sons, 1980.
4. Rodd's Chemistry of Carbon Compounds, Ed. S.Coffey and M.F.Ansell, Elsevier. 2ndEd., 1964.

## 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 biocatalysts, isolated enzyme versus whole cell systems, Enzymatic and Microbial

**Reactions:** Application in Organic Synthesis: Hydrolytic Reactions, Reductions, Oxidations, Formation of C-C Bonds, Additions and Eliminations Reactions.

**Special Techniques** Involving the Use of Enzymes and Microorganisms: Extending and Improving Biotransformations, Purified Enzymes/ Crude Enzymes, Extracts, substrate Modifications, Effects of Temperature on Enzyme Selectivity, Enzymes in Organic Solvents, Advantages of Biotransformations in Organic Solvents, Designing a Solvent System for Enzyme Catalyzed Reactions.

**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, hydroxylation 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. Down stream processing, Production of antibiotics, semi-synthetic analogues.

**BOOKS:**

- 1) Biotransformations and Bioprocesses, Doble Mukesh, Anil Kumar & Vilas Gajanan Gaikar, Marcel Dekker, New York, USA, 2004.
- 2) Biotreatment of Industrial Effluents, Doble Mukesh and Anil Kumar, Elsevier, USA, 2005.
- 3) Biotransformations in Preparative Organic Chemistry, H. G. Davies, D. R. Kelly, R. H. Green and Stanley M. Roberts, Academic Press, New York, 1989.
- 4) Bio-transformations in Organic Chemistry by Kurt Faber, Springer Verlag, Berlin, 1992.
- 5) Bioprocess Engineering Principles by Pauline M. Doran, Academic Press. 1995, ISBN-13: 978-0-12-220856-0
- 6) Bioprocess Engineering, Basic concepts by Michael L. Shuler and Fikret Kargi, Second Edition, PTR Prentice Hall. 2001, ISBN 0-13-081908-5
- 7) Medicinal Chemistry by Foye, 1990.

**REFERENCE BOOKS:**

1. Combinatorial Chemistry by Nicholas K. Terrett, Oxford Chemistry Masters, Oxford University Press, 1988.
2. Designing organic synthesis by S. Warren, John Wiley Sons 1982.
3. The Logic of Chemical Synthesis by E.J. Corey and Xue-Min Cheng, John Wiley and Sons, 1989.

**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.

**Metalloproteins - Metalloenzymes:** The characterization of metal - binding sites - Carbonic anhydrase - Carboxy peptidase - Super oxide dismutase - Structure and biochemical functions of B12 Coenzyme.

**Alkali metal transport in Biological systems:** Introduction - Coordination chemistry of alkali metal ions-Ion 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.

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

### **BOOKS :**

- 1) Inorganic Chemistry by J.E.Huheey, E.A.Keiter and R.L.Keiter, Harper collins,4th Ed.,1993 .
- 2) Advanced Inorganic chemistry by F.A.Cotton and G.Wilkinson, 5th Ed., John Wiley, 5th Ed., New York, 1988.
- 3) Structural Inorganic chemistry by A.F Wells 5th Ed., Oxford science publications, 1987.
- 4) Chemistry of the elements by N.N.Greenwood and A.Earnshaw,2 nd Ed., Butterworth-Heinemann,1997.
- 5) Inorganic Polymers, J.E. Mark, H.R.Allcock and R. West, Prentice Hall 1992.
- 6) Inorganic Reactions of biological processes by M.N.Hughes,John-Wiley, 2nd Ed., New York 1981.
- 7) Bioinorganic Chemistry by Wolfgang Kaim and B.Schwederski,John Wiley, New York , 1994.
- 8) Inorganic Biochemistry - An Introduction by J.A.Cowan, VCH, 1993.
- 9) Principles of Bioinorganic Chemistry by S.J.Lippard and J.M.Berg, University Science Books, California,1994.

### **REFERENCE BOOK:**

- 1) Advances in Boron and the Boranes, A. Reenberg and R.E. Williams, VCH,1988.

**MCH-219: FERROUS-NONFERROUS METALLURGY 4 Credits**

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(Head of the Department)  
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