COURSE OF STUDIES

FOR POST GRADUATE DEGREE IN CHEMISTRY (SEMESTER SYSTEM)

FOR THE ACADEMIC SESSION 2023-24

POST GRADUATE DEPARTMENT OF CHEMISTRY



K. K. Rehus Bleh

GOVERNMENT AUTONOMOUS COLLEGE ROURKELA

COURSE AT A GLANCE

Subject: M. Sc. in Chemistry Academic Session: 2022-24Academic Year

FIRST SEMESTER				
Course No	Course Title	Credit	Mark distribution	Mark
AECC - I	ENVIRONMENTAL STUDIES AND DIASTER MANAGEMENT Enterpunership Development	02	20+ 20 (Assign ment) + 60	100
P-101	INORGANIC CHEMISTRY-I	04	20+80	100
P-102	ORGANIC CHEMISTRY-I	04	20+80	100
P -1O3	PHYSICAL CHEMISTRY-I	04	20+80	100
P -104	INSTRUMENTAL METHODS OF ANALYSIS	04	20+80	100
P -105	INORGANIC PRACTICAL-I	02	50	50
P -106	ORGANIC PRACTICAL-I	02	50	50
	Total	22	500	600

SECOND SEMESTER				
Course No	Course Title	Credit	Mark distribution	Mark
ABCC-II	FOR NON-CORE STUDENTS Environmental bludies and Subsaster management	2	20+20 (Assig nment) + 60	100
P -201	INORGANIC CHEMISTRY-II	04	20+80	100
P -202	ORGANIC CHEMISTRY-II	04	20+80	100
P -203	PHYSICAL CHEMISTRY-II	04	20+80	100
P -204	ATOMIC & MOLECULAR SPECTROSCOPY	04	20+80	100
P -205	INORGANIC PRACTICAL-II	02	50	50
P -206	ORGANIC PRACTICAL-II	02	50	50
	Total	23 22		600

In addition to this student(s) has to take one Inter Departmental Course IDC of 3 credit offered by other departments.

THIRD SEMESTER				
Course No	Course Title	Credit	Mark distribution	Mark
AECC - II	ENTREPRENEURSHIP DEVELOPMENT	3	20+ 20 (Assignme nt) + 60	100
P -301	INORGANIC CHEMISTRY-III	04	20+80	100
P -302	ORGANIC CHEMISTRY-III	04	20+80	100
P -303	PHYSICAL CHEMISTRY-III	04	20+80	100
P -304	ANALYTICAL TECHNIQUES IN ORGANICCHEMISTRY	04	20+80	100
P -305	PHYSICAL CHEMISTRY PRACTICAL	02	50	50
P-306	INDUSTRIAL CHEMISTRY PRACTICAL	02	50	50
P-307	MOOCs one paper from Swayam or others	03		
	Total	252		600

FOURTH SEMESTER

Course No	Course Title	Credit	Mark distribution	Mark
P -401	MATERIAL & ENERGY BALANCE	04	20+80	100
P -402	INDUSTRIAL POLLUTION & ITSMANAGEMENT	04	20+80	100
P -403	ELECTIVE PAPER Process	04	20+80	100
P -404	PROJECT	04		100
P -405	ELECTIVE PAPER Medicual	04	20+80	100
	Elective Papers			
	(The student has to opt any tv	vo papers	5)	
P -403 A	INDUSTRIAL PROCESSES	04	20+80	100
P -403 B	CHEMISTRY OF NANOMATERIALS	04	20+80	100
P-405 A	MEDICINAL CHEMISTRY	04	20+80	100
P -405 B	SURFACTANTS AND DETERGENTS	04	20+80	100
	Total	20	500	500
	Total Credit	90		2300

One Non-credit course will be taken by the students during the 2 year study NCC/NSS/Sports/Yoga/Gardening/Socially Useful Productive Work (SUPW)

FIRST SEMESTER

P-101

INORGANIC CHEMISTRY-I

4 credits

UNIT-I:

Basic Concepts of Symmetry and Group Theory

Symmetry operation, symmetry element, classification of symmetry elements, definition of group, subgroup, cyclic groups, molecular point groups, group multiplication table, group generators, symmetry of platonic solids, conjugacy relation and classes, matrix representation of symmetry elements, character of a representation, reducible and irreducible representation, properties of irreducible representation.

UNIT-II:

Group Theory and Spectroscopy

Character table (explanation and significance), construction of character tables for C_{2v} , C_{3v} , C_{4v} , C_{2h} , D_{2d} and D_4 point groups, direct product, standard reduction formula, applications of group theoretical methods for selection rules in: infrared spectroscopy, Raman spectroscopy and electronic spectroscopy.

UNIT-III:

Theories of Metal-Ligand Bonding

Basic concepts of crystal field theory (CFT), molecular orbital theory (MOT): classification of metal valence orbitals into sigma symmetry, ligand group orbitals (LGOs) of sigma symmetry, LGOs of pi symmetry, molecular orbital energy level diagrams for octahedral and tetrahedral complexes, concept of ligand field theory (LFT).

UNIT-IV:

Term Diagram, Electronic Spectral and Magnetic Properties of Metal Complexes Concept of term symbols, derivation of term symbol for pn and dn configurations, Orgel diagram for dn configurations, Significance of Tanabe-Sugano diagram. Electronic spectra of metal complexes, selection rules, relaxation in selection rules, evaluation of Dq, B and beta(β) parameters for the complex with T1 ground state and A2 ground state, spectrochemical series and nephlelauxetic series, charge transfer spectra. Concept of magnetic properties of metal complexes.

TEXT BOOKS:

- 1. Chemical Applications of Group Theory by F. A. Cotton, Wiley India (P) Ltd., 3rdedn, 2009, New Delhi.
- 2. Symmetry and Spectroscopy of Molecules by K. V. Ready, New Age International Ltd. 2ndedn, 2009, New Delhi.
- 3. Symmetry and Group Theory in Chemistry by R. Ameta, New Age International Ltd., 1stedn, 2013, New Delhi.
- 4. Solid State Chemistry by D. K. Chakravarty, New Age International Limited, 1996, New Delhi.
- 5. Advanced Inorganic Chemistry by F. A. Cotton and G. Wilkinson, Wiley India (P) Ltd., New Delhi, 6th edition, 1999.
- 6. Fundamental concepts of Inorganic Chemistry (vol-5, and vol-6) by Asim K. Das and Mahua Das, CBS publishers and distributors, 2nd Edition, 2019.

REFERENCE BOOK

- 1. Inorganic Chemistry by G. L. Miessler and D. A. Tarr, Pearson Education, 3rd edn, 2004.
- 2. Inorganic Chemistry (Principles of Structure and Reactivity) by James E. Huheey, Ellen A. Keiter, Richard L. Keiter and Okhil K. Medhi Pearson Education, 4th edn, 2006.

P-102

ORGANIC CHEMISTRY I

4 credits

UNIT-I:

Aromaticity and Electronic Effects

Delocalized chemical bonding, Conjugation, Cross conjugation, Electronic effect, Aromaticity in benzenoid and non-benzenoid compounds, Huckel's rule, Alternant and non-alternant hydrocarbons, Energy levels in odd and even-alternant hydrocarbons, energy levels of π -molecular orbitals, Aromaticity of annulenes and heteroannulenes, Anti-aromaticity, Homo-aromaticity.

Classification of reactions and mechanisms, Kinetic and thermodynamic control reactions, Hammond's postulate, Transition states and intermediates in Potential energy diagrams, The Hammett equation and linear free energy relationship, Substituent and reaction constants, Hard and soft acids and bases. Effect of structure on the strengths of acids and bases.

Aliphatic Substitution Reactions

Nucleophilic substitution $-S_N 2$, $S_N 1$ and SET mechanisms. Neighboring group participation by σ and π -bonds, anchimeric assistance. Carbocation rearrangements, Nucleophilic substitution at an aliphatic trigonal, allylic and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity.

UNIT-II:

Electrophilic substitution reactions $-S_E1$, S_E2 and S_Ei mechanisms, Effect of substrate, leaving group and solvent, Reactions (hydrogen exchange, migration of double bonds, keto-enol tautomerism, halogenation, aliphatic diazonium coupling, Stork-enamine reaction).

UNIT-III:

Aromatic Substitution Reactions

Aromatic electrophilic substitution reactions – The arenium ion mechanism. Orientation and reactivity. Energy profile diagrams. Structure reactivity relationship in monosubstituted benzene, Quantitative treatment of reactivity in substrates and electrophiles. orientation in benzene and higher order rings with one or more than one substituent, Diazonium coupling, Vilsmeir - Haack reaction, Gatterman reaction, Gatterman-Koch reaction, Hoesch reaction Pechmann reaction.

Aromatic Nucleophilic Substitution – ArS_N1, ArS_N2, benzyne, Effect of substrates, leaving groups, and attacking nucleophile, Reactions: Nucleophilic displacement in areno-diazonium salts by different nucleophiles, Goldberg reaction, Schiemann reaction, Chichibabin reaction.

Free radical Substitution: Intermediates, Reaction at sp² carbon, Reactivity in aliphatic, at bridge head position and in aromatic substrates.

UNIT-IV:

General Stereochemistry

Chirality, Fischer projection and R and S notations, Threo and erythro nomenclature, E and Z nomenclature, Optical isomerism in biphenyls and allenes, Concept of Prostereoisomerism and Asymmetric synthesis, Conformation of a few acyclic molecules (alkanes, haloalkanes), Conformation of cyclic systems having one and two sp2 carbon atoms.

TEXT BOOKS:

- 1. Organic Chemistry (Second Edition), by J. Clayden, N. Greeves, S. Warren.
- 2. Organic Reactions and Their Mechanisms by P S Kalsi, New Age International Private Limited; Fifth edition, 2020
- 3. Organic Reaction Mechanisms by Raj K. Bansal, New Age International Private Limited, 2012
- 4. Mechanism and Theory in Organic Chemistry by Lowry and Richardson (Harper Row Publishers, New York)
- 5. A Guidebook to Mechanism in Organic Chemistry by Peter Sykes
- 6. Jonathan Clayden, Nick Greeves, and Stuart Warren. "Organic Chemistry," Oxford University Press, 2014.
- 7. D. Nasipuri, Stereochemistry of Organic Compounds Principles and Applications, New Age International Publishers, 3rd Edition, 2011
- 8. Stereochemistry: Conformation and Mechanism by P.S. Kalsi New Age Publishers; Tenth Edition, 2019

REFERENCE BOOKS:

- 1. Advanced Organic Chemistry: Reaction Mechanism and Structure by Jerry March (Wiley Eastern Limited)
- 2. W. Carruthares, Iain coldham, Modern Methods of Organic Synthesis South Asia Edition, Cambridge University Press, Fourth Edition, 2015.
- 3. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry Part B: Reaction and Synthesis, Springer, 5th Edition, 2010.
- 4. Stereochemistry of Organic Compounds by Ernest L. Eliel Wiley; 1st Edition, 2008

P-103

PHYSICAL CHEMISTRY I

4 credits

UNIT-I

Chemical Kinetics & Fast Reaction

Theories of reaction rates, Collision theory, Transition state theory, Arrhenius equation and the activated complex theory, Reaction between ions, Salt effect, Steady-State Kinetics, Kinetic and Thermodynamic concept of Reactions, Treatment of unimolecular reaction (Lindeman-Hinshelwood and Rice-Ramspeger-Kassel-Marcus (RRKM) theories), Dynamic chain (H₂ + Br₂ reaction, pyrolysis of CH₃CHO, Decomposition of ethane). Study of Fast reactions by relaxation, Stopped flow and Flash photolysis methods.

UNIT-II

Polymer Chemistry

Polymer-definition, Classification of polymer, Polymer structure, Number average and molecular weight average, Step growth & chain growth polymerization, Kinetics of polymerization, Stereochemistry of polymerization.

UNIT-III

Adsorption, types of adsorptions, Gibbs adsorption isotherm, Freundlich's adsorption isotherm, Langmuir's adsorption isotherm and its limitations, BET adsorption isotherm and its applications, Heat of adsorption, estimation of surface areas of solids from solution adsorption studies, Enzyme Catalysis & Heterogeneous Catalysis.

Unit-IV

Phase Rule

Concept of Equilibrium between phases, Derivation of phase rule, Ideal Solution, Liver Rule, Brief concept on one and two component system, Application of phase rule to three component systems of both solids and liquids.

TEXT

1. Chemical Kinetics by K.J. Laidler, Pearson; 3rd edition (1997)

BOOKS:

- 2. Textbook of Physical Chemistry by K L Kapoor, McGraw Hill (2014)
- 3. Principles of Physical Chemistry by B.R. Puri, L.R. Sharma, M.S. Pathania, Vishal Publishing Co, 47th Edition (2016)
- 4. Polymer Science by Gowariker, Viswanathan & Sreedhar

REFERENCE

1. Advanced Physical Chemistry by D.N. Bajpai, S. Chand; 2nd edition (1992)

BOOKS:

- 2. Atkins' Physical Chemistry by P. W. Atkins and Julio de Paula, , Oxford; 10th Edition (2014)
- 3. Reaction Kinetics by Pilling & Seakins
- 4. Physical Chemistry Through Problems by Dogra & Dogra

P-104

INSTRUMENTAL METHODS OF ANALYSIS

4 credits

UNIT-I

Atomic Absorption and Flame Emission Spectroscopy

Basic Principle of atomic absorption spectroscopy (AAS), instrumentation, atomization techniques, application of AAS, sensitivity of instruments, strengths and limitations of atomic absorption spectroscopy. Basic principle flame emission spectroscopy (FES), instrumentation, application of FES, limitations in FES.

UNIT-II

Electroanalytical Method

Polarography: principle, instrumentation, Ilkovic equation, Significance of half wave potential, application of polarography. Cyclic voltammetry: principle, instrumentation, and its application, ion selective electrodes.

UNIT-III

Thermoanalytical Methods

Thermogravimetric analysis (TGA): Principle, instrumentation, factors affecting TGA curve, derivative thermogravimetric analysis (DTGA) and application of thermogravimetric analysis, differential thermal Analysis (DTA), instrumentation of DTA and application of DTA, simultaneous study of TGA, DTA with examples. differential scanning calorimetry (DSC) and thermometric titration.

UNIT-IV

Chromatography

Principle and applications of thin layer chromatography (TLC), column chromatography (LC), gas chromatography (GC), high pressure column chromatography (HPLC).

TEXT BOOKS: 1. Analytical Chemistry (Theory and Practice) by U.N. Dash, Sultan Chand & Sons Pvt. Ltd., New Delhi, 2013.

2. Basic concept of Analytical Chemistry by S. M. Khopkar, New Age International (P) Ltd. Publishers, 3rd Edition, 2008.

3. Instrumental Methods of Chemical Analysis by Gurdeep R. Chatwal, Sham K. Anand, Himalaya Publishing House, 5th Edition, 2014.

REFERENCE BOOKS

- 1. Quantitative Analysis by Vogel, Pearson Education Ltd., New Delhi, 6th edition, 2009.
- 2. Instrumental Method of Analysis by H. Willard, L. Merritt, J. Dean & F. Settle, CBS publisher and distributors Pvt. Ltd., 7th edition, 2004.

P-105

INORGANIC CHEMISTRY PRACTICAL-I

2 credits

Analysis of an inorganic mixture containing not more than 6 radicals. The mixture will include rare earth like Tungstate, Vanadate, Molybdate and Cerium (IV). Insoluble matters and other interfering radicals will also be included. Organic radicals are excluded.

BOOKS:

- 1. Vogel's Qualitative Inorganic Analysis, 7th edition; Revised by G. Svehla.
- 2. Vogel's Text Book of Quantitative Chemical Analysis, 5th Revised by G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny.
- 3. Advanced Practical Inorganic Chemistry, 22nd edition; By Gurdeep Raj

Isolation and identification of multi-functional compounds in a mixture of two organic compounds.

BOOK:

Advanced Practical Organic Chemistry, 3/e by N K Vishnoi

SECOND SEMESTER

P-201

INORGANIC CHEMISTRY-II

4 credits

UNIT-I

Complexes of Carbon Monoxide and its Analogs

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important synthesis and reactions of metal carbonyls, carbonylate anions and carbonylate hydride, carbonyl halides; preparation, bonding and important reactions of transition metal complexes with isocyanide, cyanide, dinitrogen, carbon disulphide and nitrogen monoxides; chemistry of carbenes and carbynes.

UNIT-II

Metal Cluster and Polyacids

Concept of metal cluster, bonding in metal clusters, metal carbonyl type clusters, anionic and hydride clusters, method of synthesis, super large cluster, electron counting in medium size cluster (Wade's rule, capping rule), isolobal relationship, clusters of Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, Pt metals and their synthesis and reactions, Catalysis by metal cluster. Polyacids: definition, classification, polymerization of chromate, isopoly acids and anions, synthesis of isopoly acids, structures of isopolymolybdates, isopolytungstates and isopolyvanadates, heteropoly acids of W and Mo. Applications of isopoly and heteropoly compounds.

UNIT-III

Biomolecular Storage and Transportation of ions

Lipids, lipid bilayer, biological membranes, Ramachandran's plot, biologically important metal ions (Na, K, Mg, Ca, Cu, Fe, Zn, Co and Mo) and their functions, passive and active transport processes, Na⁺/K⁺ pump, calcium pump, ionophores, storage and transport of iron, copper and zinc, siderophores, ferritin and transferrin in regard to iron-storage and transportation.

Chemistry of porphyrin, iron porphyrins (heme proteins): hemoglobin (Hb), myoglobin (Mb) and their behavior as oxygen carrier, O₂ affinity, cooperativity and Bohr's effect, heme protein as electron carrier with particular reference to cytochrome-c and cytochrome-450, and cytochrome oxidase. Catalases and peroxidases. non-heme oxygen uptake protein (hemerythrin and hemocyanin).

Magnesium porphyrins (Chlorophyll): Photosynthesis, the light and dark reaction (Calvin cycle). Non-heme iron-sulphur protein as electron carrier, rubredoxins and ferredoxins.

UNIT-IV

Biomolecular Catalysis

Basic concepts of amino acids, peptides and proteins, structures of proteins, preliminary idea about enzyme, cofactor, co-enzyme, apoenzyme, prosthetic group, metal-activated enzyme and metalloenzyme. biological significance and mechanistic aspects of carboxypeptidase, carbonic anhydrase, blue-oxidases, non-blue oxidases, superoxide dismutase, structure and biological functions of molybdenum nitrogenase.

TEXT BOOKS:

- 1. Advance Inorganic Chemistry by F.A. Cotton, G. Wilkinson & C. Murillo, Wiley Publication, 6th edition, 1999.
- 2. Inorganic Chemistry (Principles of Structure and Reactivity) by James E. Huheey, Ellen A. Keiter, Richard L. Keiter and Okhil K. Medhi, Pearson Education, 4th edn, 2006.
- 3. Modern Aspect of Inorganic Chemistry by Emelius and Sharpe, Routledge & Kegan Paul PLC, England, 4th revised edition, 1978.
- 4. Bio-Inorganic Chemistry by Asim K Das.
- 5. Bio-Inorganic Chemistry by E. Ochia.
- 6. Bioorganic, BioInorganic and Supramolecular Chemistry by P. S. Kalsi and J. P. Kalsi.
- 7. Inorganic Chemistry (4th Edn) by Huheey, Keiter, Keiter and Medhi.
- 8. Bioinorganic and Suparmolecular Chemistry by A. Bhagi and G. R. Chatwal..

REFERENCE BOOKS

- 1. Inorganic Chemistry by G. L. Miessler and D. A. Tarr, Pearson Education, 3rd edn. 2008.
- 2. Comprehensive Coordination Chemistry, by Wilkinson, Gillarsand, Pergamon Press, 1989.

P-202

ORGANIC CHEMISTRY II

4 credits

UNIT-I

Addition Reactions

Addition to C=C multiple bonds – Electrophilic, Nucleophilic and Free radical. Reactions: Hydroboration, Michael reaction, Sharpless Asymmetric epoxidation. Addition to carbon-heteroatom multiple bonds: Mechanism and reactivity, Reactions: LiAlH4 reduction of carbonyl compounds, acids, esters, nitriles, addition of Grignard reagents to carbonyl compounds, Reformatsky reaction, Aldol condensation, Knoevenagel condensation, Perkin reaction, Mannich reaction, Wittig reaction, Stobbe reactions, Tollens reaction, Benzoin condensation.

UNIT-II

Elimination Reactions

E₁, E₂, E₁CB and E₂CB mechanisms, Orientation, Effect of substrate, base, leaving group and medium, Orientation of double bond, Sayetzeff and Hoffman rules, Pyrolytic elimination reaction, Oxidative elimination (oxidaton of alcohol by chromium, Moffatt oxidation). Reactions: Cleavage of quaternary ammonium hydroxides, Chugaev reaction, Shapiro reaction.

UNIT-III

Mechanistic Considerations

Nature of migration, migratory aptitude, memory effects. Rearrangements: Wagner-Meerwein, Favorskii, Fries, Carbene intermediate, Arndt-Eistert synthesis, Neber, Nitrene intermediates (Beckmann, Hofmann, Schmidt, Lossen, Curtius), Baeyer-Villiger, Shapiro reaction, Von-Richter, Sommelet-Hauser rearrangement.

UNIT-IV

Dynamic Stereochemistry

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

TEXT BOOKS:

- 1. Organic Chemistry (Second Edition), by J. Clayden, N. Greeves, S. Warren.
- 2. Organic Reactions and Their Mechanisms by P S Kalsi, New Age International Private Limited; Fifth edition, 2020
- 3. Organic Reaction Mechanisms by Raj K. Bansal, New Age International Private Limited, 2012
- 4. Mechanism and Theory in Organic Chemistry by Lowry and Richardson (Harper Row Publishers, New York)
- 5. A Guidebook to Mechanism in Organic Chemistry by Peter Sykes
- 6. Jonathan Clayden, Nick Greeves, and Stuart Warren. "Organic Chemistry," Oxford University Press, 2014.
- 7. D. Nasipuri, Stereochemistry of Organic Compounds Principles and Applications, New Age International Publishers, 3rd Edition, 2011
- 8. Stereochemistry: Conformation and Mechanism by P.S. Kalsi New Age Publishers: Tenth Edition, 2019

REFERENCE BOOKS:

- 1. Advanced Organic Chemistry: Reaction Mechanism and Structure by Jerry March (Wiley Eastern Limited)
- 2. W. Carruthares, Iain coldham, Modern Methods of Organic Synthesis South Asia Edition, Cambridge University Press, Fourth Edition, 2015.
- 3. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry Part B: Reaction and Synthesis, Springer, 5th Edition, 2010.
- 4. Stereochemistry of Organic Compounds by Ernest L. Eliel Wiley; 1st Edition, 2008

P-203 UNIT-I

PHYSICAL CHEMISTRY II

4 credits

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.

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UNIT-II Classical and Quantum Statistical Mechanics

Concept of probability, Starling approximations, Most probable distribution, System, Phase Space, μ -Space, Υ -Space, Liouville's Theorem, Statistical Equilibrium, Brief Concepts on Ensembles, Canonical, Grand Canonical and Micro-canonical ensembles.

Bose-Einstein statistics, Fermi-Dirac statistics and Maxwell-Boltzmann statistics

UNIT-III Partition Functions & Statistical Thermodynamic Properties of Solids

Significance of partition function, Calculation of thermodynamic properties and equilibrium constant in terms of partition functions, Evaluation of transnational, vibrational and rotational partition function for monoatomic and polyatomic ideal gases, electronic partition function.

Some thermal characteristics of crystalline solids, Classical treatment of solids, Einstein Model, Debye Modification, Limitation and modification of Debye theory.

UNIT-IV Computer Application in Chemistry

Basic structure of a computer: The CPU, the I/O devices, the internal memory, commonly used secondary storage media. Data representation: Overview of binary, octal and hexadecimal number system. The software: Concept of low level and highlevel languages, Compiler interpreter, editor, operating system concepts, salient features of Windows and LINUX operating systems. Algorithm, Flowchart, Decision-table, elements of high-level programming languages. Application of numerical methods to chemical problems.

TEXT

- 1. Text Book of Physical Chemistry by K.L. Kapoor
- BOOKS: 2. Principles of Physical Chemistry by Puri, Sharma & Pathania
 - 3. Chemical Thermodynamics by Rastogi & Mishra
 - 4. Thermodynamics for Chemists by S. Glasstone
 - 5. Molecular Thermodynamics by McQuarrir & Simon
 - 6. Statistical Thermodynamics by M. C. Gupta
 - 7. Computational Chemistry by A.C. Norris

REFERENCE

Advanced Physical Chemistry by D.N. Bajpai, S. Chand; 2nd edition (1992)
 Atkins' Physical Chemistry by P. W. Atkins and Julio de Paula, Oxford; 10th

Edition (2014)

3. Physical Chemistry Through Problems by Dogra & Dogra

P-204

BOOKS:

ATOMIC & MOLECULAR SPECTROSCOPY

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 & Rotational Spectroscopy & Raman 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.

UNIT-IV

Electron Spin Resonance Spectroscopy

Theory, instrumentation, g-values, hyperfine splitting, ESR spectra of systems with more than one unpaired electron, double resonance, ENDOR and ELDOR techniques.

TEXT

- 1. Fundamentals of Molecular Spectroscopy by C.N. Banwell
- **BOOKS:**
- 2. Fundamentals of Molecular Spectroscopy by G.M. Barrow
- 3. Molecular Spectroscopy, P.S. Sindhu

REFERENCE

1. Advanced Physical Chemistry by D.N. Bajpai, S. Chand; 2nd edition (1992)

BOOKS:

- 2. Atkins' Physical Chemistry by P. W. Atkins and Julio de Paula, , Oxford; 10th Edition (2014)
- 3. Physical Chemistry Through Problems by Dogra & Dogra
- 4. Spectroscopy Vol. I & II by Walker & Straw

P-205

INORGANIC CHEMISTRY PRACTICAL-II

2 credits

- 1. Principle of estimation of the main constituents of Brass and Portland Cement.
 - (a) Estimation of Ca and Mg in a given solution prepared from a sample of cement by EDTA method.
 - (b) Estimation of Cu in a given solution prepared from a sample of Brass.
- 2. Preparation and characterization of the following inorganic compounds:
 - (i) Tetramminecupricsulphate [Cu(NH₃)₄]SO₄ .H₂O
 - (ii) Sodium cobaltinitrite, Na₃[Co(NO₂)₆]
 - (iii) Potassium chromioxalate, K₃[Cr(C₂O₄)₃].

BOOK:

- 1. Vogel's Qualitative Inorganic Analysis, 7th edition; Revised by G. Svehla.
- 2. Vogel's Text Book of Quantitative Chemical Analysis, 5th Revised by G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny.
- 3. Advanced Practical Inorganic Chemistry, 22nd edition; By Gurdeep Raj

P-206

ORGANIC CHEMISTRY PRACTICAL-II

2 credits

- 1. Preparation of benzoin, benzil and benzillic acid from benzaldehyde.
- 2. Preparation from p-idotoluene from p-toluidene.
- 3. Preparation of ethyl acetoacetate from ethyl acetate.
- 4. Estimation of nitrogen by Kjeldahl method.
- 5. Estimation of keto group by gravimetric method.
- 6. Dibenzalacetone from benzaldehyde.
- 7. Cannizaro reaction 4-chloro benzaldehyde as substrate.
- 8. Grignard reaction synthesis of triphenyl methanol from benzoic acid.

BOOK:

Advanced Practical Organic Chemistry, 3/e by N K Vishnoi

Biophysics, Nanoscience & Computational design INTERDISCIPLINARY COURSE ON CHEMISTRY 3 credits Ar interdisciplinary

IDC

UNIT-I

MOLECULAR BIOPHYSICS

Basic ideas on structure and conformation of simple molecules, structural features of proteins, nucleic acids, carbohydrates and lipids. Aspects of biomolecular forces, Higher order structural organization of proteins and nucleic acid, Basic thermodynamics, ligand binding and cooperativity in biological systems, kinetics, diffusion and sedimentation.

UNIT II

NANOMATERIALS FOR ENERGY CONVERSION AND STORAGE MATERIALS

Nanomaterials for Solar energy conversion systems, Principles of photovoltaic energy conversion (PV), Structural characteristics and concepts. Types of Photovoltaic cells, Physical concept of photovoltaic cells. Organic solar cells, Dye- Sensitized Solar cells, Organic-Inorganic Hybrid solar cells, Device fabrication techniques and characterizations.

UNIT III

COMPUTATIONAL DESIGN ON DRUGS AND FUNCTIONAL MATERIALS

Structure representation: Building of small molecules, co-ordinate system for structure representation, Building of Biopolymers and oligopeptides. Conformational analysis, Molecular docking, Structure and features of conducting and semiconducting organic materials, Machine learning approach as future prospect.

BOOK:

- 1. Principles of Biochemistry: International Edition, David Nelson and Michael Cox, WH Freeman; 7th ed. 2017.
- 2. Biophysical chemistry, Charles R Cantor and Paul R Schimmet, WH Freeman, 1980
- 3. Organic Photovoltaics- materials, device Physics and Manufacturing Technologies, (eds. C. Brabec, V Dyakonov, U Scherf) 2 nd Ed. Wiley-VCH, Germany, 2014.
- 4. Solar cells: Operating principles, technology and system applications by Martin A Green, Prentice Hall Inc, Englewood Cliffs, NJ, USA, 1981.
- 5. Introduction to Computational Chemistry by Frank Jensen, Wiley Publication.
- 6. Andrew R Leach, Molecular Modeling: Principles and Applications, 2nd Ed., Prentice Hall, 2001

THIRD SEMESTER

P-301

INORGANIC CHEMISTRY-III

4 credits

UNIT-I

Substitution Reactions in Octahedral Complexes

Nature of substitution reactions, kinetic application of Crystal Field Theory, acid hydrolysis of octahedral Co(III) complexes with reference to effect of charge, chelation, steric crowding & effects of leaving group, base hydrolysis of octahedral Co(III) complexes: Conjugate base mechanism, test of conjugate base mechanism, anation reaction, substitution reaction without cleavage of metal-ligand bond.

UNIT-II

Substitution Reactions in Square Planar Complex and Redox Reactions

Thermodynamic and kinetic stability, trans effect and its synthetic applications, theories of trans effect (polarization & π -bonding theories), factors affecting the rate law and reaction profile (leaving group, steric group, charge, electrophillic catalysis, nucleophile and temperature). Redox reactions: electron tunneling hypothesis, concept of Marcus-Hush theory, atom transfer reactions, one and two electron transfer, complementary and non-complementary reactions, inner sphere and outer sphere reactions, electron transfer through extended bridges, concept of hydrated electron.

UNIT-III

Nuclear Chemistry

Nuclear stability, magic numbers, radioactivity, general characteristics of radioactive decay particles, decay kinetics, nuclear reaction, Bethe's notation, types of nuclear reaction, nuclear cross section, compound nuclear theory, nuclear fission, liquid drop model, shell model, hard core preformation theory, fission fragments and their mass distribution, charge distribution, ionic charge of fission fragments, working principle of nuclear reactor, concept of nuclear fusion, concept of boron-neutron capture therapy.

UNIT-IV

Solid State Chemistry

General idea of crystal lattice, unit cell, classification of crystals, crystal planes, Miller indices, Bragg's law and applications, determination of cubic crystal structure from systematic absences in diffraction pattern, perfect and imperfect crystals, point defects, stoichiometry defects, Schottky defects and Frenkel defects, thermodynamics of Schottky and Frenkel defects, bonding in ionic solids, colour centers, non-stoichiometry defects, band structure of solids.

TEXT

1. Mechanisms of Inorganic Reactions by F. Basolo and R. G. Pearson.

BOOKS:

- 2. Inorganic Chemistry by Asim K Das.
- 3. Inorganic Chemistry by Cotton and Wilkinson (4th Edn).
- 4. Essentials of Nuclear Chemistry by H. J. Arniker
- 5. Solid State Chemistry by D. K. Chakravarty, New Age International Limited, 1996, New Delhi.

REFERENCE BOOKS

- 1. Solid State Chemistry and its Applications by A.R. West, Wiley, 1989, 2nd edition, Singapore.
- 2. Principles of the Solid State by H.V. Keer, Wiley Eastern. Limited, 1993, New Delhi.

P-302

ORGANIC CHEMISTRY III

4 credits

UNIT-I

Organic Redox Reaction

Oxidation: Oxidation of hydrocarbons, oxidation of alcohols by various reagents, oxidation of carbon-carbon double bonds to diols and epoxides, Chromium (VI), Manganese (VII) oxidants, Oxidation with peracids, with hydrogen peroxide, with singlet oxygen. with iodobenzene diacetate, and thallium (III) nitrate.

<u>Reduction</u>: Catalytic hydrogenation, selectivity of reduction, Reduction by hydride transfer reagents: Aluminium alkoxid, Sodium borohydride (NaBH₄), dissobutylaluminium hydride, Sodium cyanoborodydride, Lithium trialkylborohydride, reduction with hydrazine, reduction with trialkyltinhydride, the Birch reduction, the Wolff-Kischner reduction, the Cannizarro reduction, the Resemmend reduction.

UNIT-II

Pericyclic Reaction and Photochemistry

Pericyclic reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann rules, Correlation diagrams and FMO approach. Electrocyclic reactions - Conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloaddition reactions - suprafacial and antarafacial additions, 4n and 4n+2 systems, thermal and photochemical processes, 1,3 dipolar cycloadditions and cheletropic

reactions. Sigmatropic rearrangements - [i,j] shifts of C-H and C-C bonds; Sommelet-Hauser, Claisen, thio-Claisen, Cope and aza-Cope rearrangements. Ene reaction. Photochemical processes: Fluorescence, Phosphorescence, excimers and exciplex formation, Photochemical reactions: Cis-Trans Isomerization, photochemical dissociation, Reduction of ketones, Paterno-Buchi reaction, Norrish type I and II reactions, Di-π-methane rearrangement, Photochemistry of arenes, Barton reaction.

UNIT-III

Reagents in Organic Synthesis

Gilman's reagent, Lithium dimethyl cuprate, Lithium diisopropyl amide, DCC, 1,3-Dithiane, Trimethyl silyl iodide, Tri-n-butyl tin hydride, Osmium tetroxide, Selenium dioxide, Phase transfer catalysis (Crown ether, Merrifield resin, Wilkinson's catalyst), Dichloro dicyano benzoquinone (DDQ).

UNIT-IV

Retrosynthetic Approach

Synthetic design: Introduction, Retrosynthetic approach, Terminology in Retro synthetic analysis, One group disconnection, (alcohol, carbonyl compound, olefins and acids), Two group disconnections (β -hydroxy compounds, α , β -unsubstituted carbonyl compounds, 1,3-dicarbonyl compounds, 1,5 dicarbonyl compounds), Synthesis of some organic molecules by disconnection approach.

TEXT BOOKS:

- 1. Reactions, Rearrangements and Reagents by S.N. Sanyal, Bharati Bhawan Publishers & Distributors; Fourth edition, 2019
- 2. Organic Reaction Mechanisms by Raj K. Bansal, New Age International Private Limited, 2012
- 3. Synthetic Approaches in Organic Chemistry, R.K. Bansal, Narosa Publishing House, India, 1996
- 4. Jonathan Clayden, Nick Greeves, and Stuart Warren. "Organic Chemistry," Oxford University Press, 2014.
- 5. Organic Reactions and Orbital Symmetry by Gilchrist and Storr, Cambridge University Press; 2nd Edition 1979
- 6. Mechanism and Theory in Organic Chemistry by Lowry and Richardson (Harper Row Publishers, New York)
- 7. Photochemistry and Pericyclic Reactions by Jagdamba Singh and Jaya Singh, New Age; 3rd Edition, 2012
- 8. Stuart Warren and Paul Wyatt, Organic synthesis, the disconnection approach, 2nd edition, Wiley, 2012.

REFERENCE BOOKS

- 1. W. Carruthares, Iain coldham, Modern Methods of Organic Synthesis South Asia Edition, Cambridge University Press, Fourth Edition, 2015.
- 2. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry Part B: Reaction and Synthesis, Springer, 5th Edition, 2010.
- 3. J. March and M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edition, Wiley, 2013.
- 4. I. L. Finar, Organic Chemistry Vol. I & Vol. II, Longman (Cambridge), 2011.

P-303

PHYSICAL CHEMISTRY III

4 credits

UNIT-I

Exact Quantum Mechanical Results

The Schrodinger equation and the postulates of quantum mechanics, Elementary application of the Schrodinger equation, Particle in a box, Harmonic oscillators, Rigid rotator and hydrogen atom.

UNIT-II

Approximate Methods & Angular Momentum

The variation theorem, Time independent perturbation of non-degenerate systems, Application of Variation Method and Perturbation Theory to the He atom. Ordinary angular momentum, generalized angular momentum, Eigen functions for angular momentum, Addition of angular momentum.

UNIT-III

Chemical Bonding in Diatomics

Born-Oppenheimer Approximation, Molecular Orbital Theory and its Applications, Valence Bond Theory and its Applications, LCAO-MO Theory.

UNIT-IV

Orbital Approximation Methods

Huckel theory of conjugated systems (Ethylene, Allyl systems, butadiene, cyclopropenyl, cyclobutadiene, bicyclobutadiene, H_3^+ , H_3 and H_3^-), Calculation of bond order, charge density, free valence index, Application of group theory for the simplification of MO determinants of 1,4- butadiene and naphthalene.

TEXT

BOOKS:

1. Introductory Quantum Chemistry, A.K. Chandra

2. Fundamentals of Quantum Chemistry, R.K. Prasad

3. Notes on Molecular Orbital Calculations by J.D. Roberts

REFERENCE BOOKS:

1. Quantum Mechanics, Volume 2: Angular Momentum, Spin, and Approximation Methods, 2nd Edition, Claude Cohen-Tannoudji, Bernard Diu, Franck Laloë; Wiley-VCH, 2019

The Chemical Bond: Fundamental Aspects of Chemical Bonding, Eds. Gernot Frenking, Sason Shaik; Wiley-VCH, 2014

P-304

ANALYTICAL TECHNIQUES IN ORGANIC CHEMISTRY

4 credits

UNIT-I

Nuclear Magnetic Resonance

Magnetic properties of nuclei, Theory of magnetic nuclear resonance with special reference to proton, Instrumentation, Chemical shift, Simple spin-spin interaction, Shielding effects, Diamagnetic anisotropy, NOE, ¹³C, ¹⁵N, ¹⁹F, ³¹P NMR (preliminary idea).

UNIT-II

Mass Spectrometry

Introduction, Mass spectrum, Determination of molecular formulae, molecular ions, Parent peak, Base peak, Use of molecular fragmentation, McLafferty rearrangement, Mass spectra of some classes of compounds (hydrocarbons, alcohols, phenols, ketones, aldehydes, acids and esters)

UNIT-III

Spectroscopic Identification of Organic Compounds

Problems involving identification of organic compounds using UV, IR, NMR and Mass spectroscopy.

UNIT-IV

Optical Rotatory Dispersion and Circular Dichroism

Plane polarized and circularly polarized lights, Circular birefringence and circular dicroism, ORD, Cotton effect, Rotatory Dispersion of ketones, the Octant rule, Axial haloketone rule.

TEXT **BOOKS:**

- 1. Introduction to Spectroscopy by Donald L. Pavia, Gary M. Lampman, George S. Kriz, and James R. Vyvvan, Cengage Learning India Private Limited; 2015
- 2. R.M. Silverstein, G. C. Bassler, T. C. Morril, Spectrometric identification of Organic Compounds, John Wiley & Sons, Inc. 2010
- 3. D. Nasipuri, Stereochemistry of Organic Compounds Principles and Applications, New Age International Publishers, 3rd Edition, 2011
- 4. Spectroscopic Identification of Organic Compounds: Silverstein & Basselor, Wiley: 8th edition, 2014

REFERENCE **BOOKS** P-305

- 1. Spectroscopy of Organic Compounds, by P S Kalsi, New Age International, 2007
- 2. Basic ¹H- and ¹³C NMR spectroscopy, by M. Balci, Elsevier, 2005

PHYSICAL CHEMISTRY PRACTICAL

2 credits

- Determination of ionization constants of weak acids and verification of Oswald's 1. Dilution law.
- Conductometric titration of a mixture of HCl+CH₃COOH with NaOH 2.
- 3. Base hydrolysis of ethylacetate conductometrically.
- Potentiometric titration of strong acid with strong base. 4.
- Verification of Beer's Lambert Law and unknown concentration determination. 5.
- Simultaneous estimation of Mn and Cr in a solution of KMnO₄ and K₂Cr₂O₇. 6.
- To estimate metal ions by spectrophotometric titration. 7.
- Determine the pK value of an acid-base indicator.
- 9. Determination of rate constant of acid hydrolysis of ethyl acetate.
- 10. Determination of unknown dextrose solution by polarimetry
- 11. Study of inversion of cane sugar in acid medium by polarimetry.
- 12. Adsorption of CH₃COOH on activated charcoal and verification of Freundlich's & Langumir's adsorption isotherm.
- 13. Determination of association constants of CH3COOH by distribution method between water and toluene.
- 14. To study the rate of acid catalysed iodination of acetone in presence of excess acid and acetone.
- 15. Determination of ionisation constants of multibasic acid using a pH meter.

Books:

- 1. Practical Physical Chemistry by B. Viswanathan & P. S. Raghavan, Viva Books
- 2. Experimental Physical Chemistry by R.C. Das & B. Behera, McGraw-Hill Education

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P-306

INDUSTRIAL CHEMISTRY 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. Preparation of indigo from anthranilic acid.
- 5. Preparation of cinnamic acid from benzaldehyde.
- 6. Preparation from flavone from o-hydroxy acetophenone.
- 7. Estimation of sulfur in isothiouronium chloride prepared from thiourea.
- 8. Separation of components from a mixture by TLC and column chromatography.

TEXT BOOK:

FOURTH SEMESTER (Core Courses)

P-401 MATERIAL & ENERGY BALANCE

4 credits

UNIT-I:

Material Balances Without Chemical Reactions

Process Flow-Sheet, Material Balances, Recycling Operations, Material Balances of Unsteady State Operations.

UNIT-II:

Material Balances Involving Chemical Reactions

Definition of Terms, Electrochemical Reactions, Recycling, Parallel and Bypassing Operations, Metallurgical Applications

UNIT-III:

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, Thermochemistry of Mixing Process, Dissolution of Solids, Liquid-Liquid Mixtures

UNIT-IV:

Stoichiometry and Unit Operations

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

TEXT BOOKS:

- 1. G.V. Reklaitis, Introduction to Material and Energy Balances, 1st Edition, John Wiley & Sons, 1983.
- 2. V.V. Veverka and F. Madron, Material and Energy Balancing in the Process Industries: From Microscopic Balances to Large Plants, 1st Edition, Elsevier, 1997.
- 3. B.I. Bhatt and S.B. Thakore, Stoichiometry, 5th Edition, Tata McGraw Hill, 2010.

REFERENCE BOOKS

- 1. A.E. Morris, G. Geiger, and H.A. Fine, Handbook on Material and Energy Balance Calculations in Material Processing, 3rd Edition, John Wiley & Sons, 2011.
- 2. C. Oloman, Material and Energy Balances for Engineers and Environmentalists, 3rd Edition, Imperial College Press, 2009.

P-402

INDUSTRIAL POLLUTION & ITS MANAGEMENT

4 credits

UNIT-I

Basics of Industrial Pollution

Concept and definition of Industrial pollution, Environment and its classification, Factors influencing environment, Components of Environment; Bio-geochemical cycles; Hydrological cycle, Gaseous cycles (Oxygen cycle, CO₂ cycle, Nitrogen cycle), Sedimentary cycles (Sulfur cycle, Phosphorous cycle); Effects of Industries on the environment; Environmental degradation.

UNIT-II

Industrial Air Pollution

History of major industrial air pollution episodes. Types and classification of Industrial air pollutants. Characterization of gaseous effluents of major industries (thermal power plant, steel, cement, aluminum, paper, fertilizer) and their health effects. Permissible limit and ambient air quality, Methods for control of gaseous air pollutants (Combustion, Absorption and Adsorption). Methods for control of particulate air pollutants (Mechanical device, Filtration, Dry scrubber, Electrostatic precipitator).

UNIT-III

Industrial Water Pollution

History of major industrial water pollution episodes, Classification and types of Industrial water pollutants, Characterization of some liquid effluents of major polluting industries (Paper Mills, Sugar industry, Iron and steel and Textile) and their health effects, Water quality standard: Drinking water quality standard, Irrigation water standard and effluent standard, methods of treatment of industrial waste water: Preliminary treatment, primary treatment, (Sedimentation, equalization and neutralization etc.), secondary treatment (Activated sludge technique and Trickling filter) tertiary treatment methods for waste water treatment (Evaporation, Ion exchange, Adsorption, Electrodialysis, Electrolytic recovery, reverse osmosis).

UNIT-IV

Industrial Solid Wastes

Classifications and types of Industrial solid wastes, Generation, disposal and management of industrial solid wastes with special reference to fly ash, red mud, heavy metals (Mercury, Lead, Arsenic, Cadmium), other organic solid wastes and radio-active wastes. Industrial sources of noise, Loudness on Decibel scale, noise levels in decibel scale, effect of noise on human health, prevention and control of industrial noise pollution.

TEXT BOOKS

- 1. Industrial Pollution and Management by Arvind Kumar, APH Publishing Corporation, New Delhi.
- 2. Industrial Pollution and its Management by P.C. Trivedi, Avishkar Publishers & Distributors, Jaipur
- 3. Pollution Control in Process Industries by S.P. Mahajan, Tata McGraw Hill Publishing Company, New Delhi
- 4. Environmental Engineering by G Kiely, Tata McGraw Hill Publishing, Company, New Delhi.

REFERENCE BOOKS

1. Environmental Pollution and Control, 4th ed. by J. Jeffrey Peirce, P. Aarne Vesilind, Ruth F. Weiner, Elsevier Publication

P-405

PROJECT

4 credits

Each-student shall-carry out project-work in industries/institutions.—The-findings of the project work should be submitted in the form of a dissertation for evaluation by a Board of Examiners.

Elective Papers

(The student has to opt any two papers)

P-403A

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.[10]

UNIT-II

Oil Based Industries & Surface-Active Agents

Oils and fats: Solvent extraction of oils, hydrogenation of oil, use of oil in the manufacturing of soap, paints and varnishes.

Classification of surface-active agents and manufacturing of detergents used for cleansing purpose.

UNIT-III

Fermentation Industries

A general discussion on fermentation conditions, manufacturing of penicillin, Alcoholic beverages, ethanol from molasses and starchy material

UNIT-IV

Pesticides and Pharmaceutical Industries

DDT manufacture, BHC manufacture, 2,4-D manufacture, parathion manufacture, pharmaceutical industry

TEXT 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

P-403B

CHEMISTRY OF NANO MATERIALS

4 credits

UNIT-I:

Semiconductors and Devices

Conducting and semiconducting organic materials. Synthesis and characterizations of organic semiconductors, Conducting and semiconducting materials and insulator, Band gap engineering. Doping of semiconductors. Application of carbon-based materials. Electronic devices and coating.

UNIT-II:

Nanomaterials for Energy Conversion and Storage Materials

Nanomaterials for Solar Energy Conversion Systems. Principles of photovoltaic energy conversion (PV), Structural characteristics and concepts. Types of photovoltics Cells, Physical concept of photovoltaic cells, Organic solar cells, Dye-Sensitized Solar Cells, Organic-Inorganic Hybrid solar cells. Device fabrication techniques and characterizations, Applications of nanomaterials in in agriculture, food, textile, cosmetics. Current status and future trends.

UNIT-III:

Nanostructured Materials

Intermolecular forces during the formation of nanostructured materials, Structure and features of conducting and ferroelectric materials, structure and features of ferroelectric materials, dielectric properties, piezo and inverse piezoelectric effects, ceramic materials, organic/inorganic hybrid materials and their fabrications and applications.

UNIT-IV

Polymers and their Applications

Stress-strain behavior, High temperature resistant organic/inorganic polymers, effect of chain flexibility and other steric factors, entropy and heat of fusion, glass transition temperature, relationship between Tm and Tg. Effect of molecular weight on polymer properties and their applications. Synthetic procedure commercial polymers (polycarbonate, polyurethane, polymethylmethacrylate, polyethyleneterpthalate, Nylon, polystyrene), Fire retarding and biomedical polymers

TEXT BOOKS

- 1. Organic Photovoltaics Materials, Device Physics and Manufacturing Technologies, (eds. C. Brabec, V. Dyakonov, U. Scherf), 2nd Ed., Wiley-VCH, Germany, 2014.
- 2. Solar cells: Operating principles, technology and system applications by Martin A Green, Prentice Hall Inc, Englewood Cliffs, NJ, USA, 1981.
- 3. Semiconductor for solar cells, H J Moller, Artech House Inc, MA, USA, 1993.
- 4. Recent Literatures and Reviews

REFERENCE BOOKS

1. Solis state electronic device, Ben G Streetman, Prentice Hall of India Pvt Ltd., New Delhi 1995.

P-405A

MEDICINAL CHEMISTRY

4 credits

UNIT-I

Overview of drug action and Modern Drug Development Process

Definition of drugs, types of pharmacological action of drugs, classification of drugs based on their origin, Drug action, Factors affects ADMET, Modern Drug Development process, Initial steps in drug discovery process, Screening of model organism, parameters involved in drug design physicochemical ionization, H-bonding, chelation.

UNIT-II

Pharmacokinetics and Pharmacodynamics

Introduction, Kinetics of ADME, Methods of assessing major physicochemical properties of compounds, Biochemistry of enzymes, Allosteric enzymes, Roles of enzymes in metabolism, Receptors, their types, location, isolation, transduction mechanism.

UNIT-III

Strategies for Synthesis of Candidate Drug

- 1. Target selection
- 2. Retro synthesis (the disconnection approach consecutive versus conversion synthesis including LHASA, strategic bond approach, strategic bond in ring approach, degradation of techniques in, synthetic design of venalflaxin, doxopicomine, clobutinol, nisoxetine, bropirimine.

UNIT-IV

Drug and their Applications

Chemotherapy of cancer: veincristine and vinblastine and taxol, drug related hormones insulin, vasopressin and oxitosin, prostaglandin, histamine, antiparkinosin agents antialzehimer agents, antirheumatics and antigout agents.

4. An Introduction to Medicinal Chemistry, Dr. Bijoy Kundu, Wiley, First Edition, 2020

TEXT

1. Introduction to the Principles of Drug Design by Smith and Williams.

BOOKS:

- 2. Principle of Biochemistry by A.L. Lehninger, D.L. Nelson & Michael M Cox.
- 3. Organic Chemistry by J. Clayden, N. Greeves, S Warrens, P. Wothers.

REFRENCE

1. Medicinal Chemistry by Alfred Burger.

BOOKS:

2. Strategy of Drug Design by Purcell.

P-405 B

SURFACTANTS & DETERGENTS

4 credits

UNIT-I

Structural Aspects of Surfactants

Surfactants, Classification (Anionic surfactants, Cationic head surfactant, Zwitterionic surfactants, Nonionic surfactant, Biosurfactants, Gemini surfactant, double tailed surfactant, Bolaform), Synthesis of Surfactant, Behaviour of Surfactants in aqueous and nonaqueous solution, Different types of interactions, Surface activity, Surface tension, Factors for organization of surfactants and types of organized assemblies, Hydrophobic interactions, electrostatic interactions, Critical micellar concentration (CMC), Factors affecting CMC, Methods of CMC determination. Aggregation number, Shape and Size of micelle.

UNIT-II

Application of Surfactant

Spectroscopic investigation and analytical methods, determination of polarity of micelle, structures of micelle, Determination of aggregation number, Industrial Applications of surfactants, Beneficiation of minerals, micellar catalysis, Drug delivery, Wetting, Dispersion and foaming.

UNIT-III

Structural Aspects of Detergents

Detergents, Principal groups of synthetic detergents, Anionic detergents, Cationic detergents, Non-ionic detergents, Amphoteric detergents, Industrial methods of preparation of Detergents, Concept of hard and soft water, Removal of hardness of water, Oil and fat, General idea of Suds regulators, builders, additives.

UNIT-IV

Application of Detergents

Manufacture of Shampoos. theories of glyceride structure, Hydrolysis of glycerides, Use of oil in the manufacturing of soap, Principle of soap cleaning, Analysis of soaps as per BIS standards, use of enzymes in detergents, Catalytic hydrogenation of oil, Recovery of Nickel from hydrogenated oil product.

BOOKS:

- 1. Industrial Chemistry by B. K. Sharma, 9th Edn.
- 2. The Manufacture of Soaps other Detergents and Glycerin Edited by Edgar Woollatt.
- 3. Synthetic Detergent Edited by Milwidsky.
- 4. Bailey's Industrial Oil and Fat Products Vol-1 (4th Edition) Edited by Daniel Swern.
- 5. Soaps & Detergent Edited by K.S. Parasuram.
- 6. Surfactants and Interfacial Phenomenon by M.J. Rosen
- 7. Catalysis in Micellar and Macromolecular Systems BY E.J. Fendler and J.H. Fendler