MANONMANIAM SUNDARANAR UNIVERISTY,
TIRUNELVELI-12

SYLLABUS

PG - COURSES – AFFILIATED COLLEGES

Course Structure for M. Sc. Chemistry
(Choice Based Credit System)
(with effect from the academic year 2023-2024 onwards)

Semester-II				
Part	**Subject Status**	**Subject Title**	**Subject Code**	**Credit**
3	Core	ORGANIC REACTION MECHANISM II		4
3	Core	PHYSICAL CHEMISTRY		4
3	Practical	ORGANIC CHEMISTRY PRACTICAL - II		3
3	Practical	INORGANIC CHEMISTRY PRACTICAL - I		3
3	Elective	MEDICINAL CHEMISTRY/GREEN CHEMISTRY		3
3	Elective	BIO INORGANIC CHEMISTRY/MATERIAL SCIENCE		3
3	SEC – I	COMPUTATIONAL CHEMISTRY		2

Total Marks: 100 Internal Exam: 25 marks + External Exam: 75 marks

A. **Scheme for internal Assessment**:
Maximum marks for written test: **15 marks**
3 internal tests, each of **I hour** duration shall be conducted every semester.
To the average of the **best two** written examinations must be added the marks scored in. The **assignment** for 5 marks and Seminar for 5 marks

The break up for internal assessment shall be:
Written test- 15 marks; Assignment -5 marks; Seminar-5 Marks Total - 25 marks

B. Scheme of External Examination
3 hrs. examination at the end of the semester
A – Part : 1 mark question two - from each unit
B – Part : 5 marks question one - from each unit
C – Part : 8 marks question one - from each unit

➢ Conversion of Marks into Grade Points and Letter Grades

S.No.	Percentage of Marks	Letter Grade	Grade Point	Performance
1	90 - 100	O+	10	Outstanding
2	80 - 89	O	9	Excellent
3	70 - 79	A+	8	Very Good
4	60 - 69	A	7	Good
5	55 - 59	B+	6	Above Average
6	50 - 54	B	5	Pass
7	0 - 49	RA	-	ReAppear
8	Absent	AA	-	Absent

➢ Cumulative Grade Point Average (CGPA)

$$\mathbf{CGPA} = \frac{\mathbf{\Sigma\,(GP \times C)}}{\mathbf{\Sigma C}}$$

- **GP** = Grade point, **C** = Credit
- CGPA is calculated only for Part-III courses
- CGPA for a semester is awarded on cumulative basis

➢ Classification

a) First Class with Distinction : CGPA $\geq$ 7.5*****
b) First Class : CGPA $\geq$ 6.0
c) Second Class : CGPA $\geq$ 5.0 and $<$ 6.0
d) Third Class : CGPA $<$ 5.0

ORGANIC REACTION MECHANISM - II

Objectives of the course

- To understand the mechanism involved in various types of organic reactions with evidences.
- To understand the applications of synthetically important reagents.
- To design synthetic routes for synthetically used organic reactions.

UNIT-I:

Elimination and Free Radical Reactions: Mechanisms: E2, E1, and E1cB mechanisms. Syn- and anti-eliminations. Orientation of the double bond: Hoffmann and Saytzeff rules. Reactivity: Effect of substrate, attacking bases, leaving group and medium. Stereochemistry of eliminations in acyclic and cyclic systems, pyrolytic elimination. Long lived and short-lived radicals – Production of radicals by thermal and photochemical reactions, Detection and stability of radicals, characteristics of free radicals, Reactions of radicals: polymerization, addition, halogenations, aromatic substitutions, rearrangements. Reactivity: Reactivity on aliphatic, aromatic substrates, reactivity in the attacking radical, effect of solvent.

UNIT-II:

Oxidation and Reduction Reactions: Mechanisms: Direct electron transfer, hydride transfer, hydrogen transfer, displacement, addition-elimination, oxidative and reductive coupling reactions. Mechanism of oxidation reactions: Dehydrogenation by quinones, selenium dioxides, ferricyanide, mercuric acetate, lead tetraacetate, osmium tetroxide, Reactions involving cleavage of C-C bonds - cleavage of double bonds, oxidative decarboxylation, allylic oxidation, oxidation by chromium trioxide-pyridine, DMSO-Oxalyl chloride (Swern oxidation) and Corey46 Kim oxidation, dimethyl sulphoxide- dicyclohexyl carbodiimide (DMSODCCD). Mechanism of reduction reactions: Wolff-Kishner, Clemmenson, Rosenmund, reduction with Trialkyl and triphenyltin hydrides, Homogeneous hydrogenation, Hydroboration with cyclic systems, MPV and Bouveault-Blanc reduction.

UNIT-III:

Rearrangements:

Rearrangements to electron deficient carbon: Pinacol-pinacolone and semi-pinacolone rearrangements - applications and stereochemistry, Wagner-Meerwein, Demjanov, Dienone-phenol, Benzilic acid and Wolff rearrangements. Rearrangements to electron deficient nitrogen: Hofmann, Curtius, Schmidt, Lossen, Beckmann and abnormal Beckmann rearrangements. Rearrangements to electron deficient oxygen: Baeyer-Villiger oxidation and Dakin rearrangements. Rearrangements to electron rich atom:

Favorskii, Quasi-Favorskii, Stevens, [1,2]-Wittig and [2,3]-Wittig rearrangements. Fries and Photo Fries rearrangement. Intramolecular rearrangements: Claisen, abnormal Claisen, Cope, oxy- Cope and Benzidine rearrangements.

UNIT-IV: Addition to Carbon Multiple Bonds:

Mechanisms: Addition to carbon-carbon multiple bonds: Addition reactions involving electrophiles, nucleophiles, free radicals, carbenes and cyclic mechanisms-Orientation and reactivity, hydrogenation of double and triple bonds, Michael reaction, addition of oxygen and Nitrogen Addition to carbon-hetero atom multiple bonds: Mannich reaction, acids, esters, nitrites, addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, Wittig reaction, Prins reaction. Stereochemical aspects of addition reactions. Mechanism of condensation reactions involving enolates –Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

UNIT-V: Reagents and Modern Synthetic Reactions:

Lithium diisopropylamine (LDA), Sodium cyanoborohydride (NaBH3CN), meta-Chloroperbenzoic acid (m-CPBA), Dimethyl aminiopyridine (DMAP), n-Bu3SnD, Triethylamine (TEA), Diethylazodicarboxylate (DEAD), N-bromosuccinimide (NBS), Trifluoroacetic acid (TFA), Phenyl trimethyl ammonium tribromide (PTAB). Diazomethane and Zn-Cu, Diethyl maleate (DEM), Copper diacetylacetonate (Cu(acac)2), TiCl3, NaIO4, Pyridinium chlorochromate (PCC), Pyridinium dichromate (PDC), Meisenheimer complex. Suzuki coupling, Heck reaction, Negishi reaction, Baylis-Hillman reaction.

Recommended Text

1. J.March and M. Smith, Advanced Organic Chemistry, 5th ed., John-Wiley and Sons. 2001.
2. E.S. Gould, Mechanism and Structure in Organic Chemistry, Holt, Rinehart and Winston Inc., 1959.
3. P.S. Kalsi, Stereochemistry of carbon compounds, 8thedn, New Age International Publishers, 2015.
4. P.Y.Bruice, Organic Chemistry, 7thedn.,Prentice Hall, 2013.
5. R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee Organic Chemistry, 7th edn., Pearson Education, 2010.

Reference Books

1. S.H. Pine, Organic Chemistry, 5thedn, McGraw Hill International Editionn, 1987.
2. L.F. Fieser and M. Fieser, Organic Chemistry, Asia Publishing House, Bombay, 2000.

3. E.S. Gould, Mechanism and Structure in Organic Chemistry, Holt, Rinehart and Winston Inc., 1959.
4. T.L. Gilchrist, Heterocyclic Chemistry, Longman Press, 1989.
5. J.A. Joule and K. Mills, Heterocyclic Chemistry, 4thed., John- Wiley, 2010.

Website and e-learning

1. https://sites.google.com/site/chemistryebookscollection02/home/organicchemistry/organicsource
2. https://www.organic-chemistry.org/

PHYSICAL CHEMISTRY-I

Objectives of the course

- To recall the fundamentals of thermodynamics and the composition of partial molar quantities.
- To understand the classical and statistical approach of the functions.
- To compare the significance of Maxwell-Boltzman, Fermi-Dirac and Bose-Einstein statistics.
- To correlate the theories of reaction rates for the evaluation of thermodynamic parameters.
- To study the mechanism and kinetics of fast reactions.

UNIT-I:

Classical Thermodynamics: Partial molar properties- Chemical potential, Gibb's-Duhem equation-binary and ternary systems. Determination of partial molar quantities. Thermodynamics of real gases - Fugacity- determination of fugacity by graphical and equation of state methods-dependence of temperature, pressure and composition. Thermodynamics of ideal and non-ideal binary mixtures, Duhem - Margulus equation, applications of ideal and non-ideal mixtures. Activity and activity coefficients-standard states - determination-vapour pressure, EMF and freezing point methods.

UNIT-II:

Statistical thermodynamics: Introduction of statistical thermodynamics, concepts of thermodynamic and mathematical probabilities-distribution of distinguishable and non-distinguishable particles. Assemblies, ensembles, canonical particles. Maxwell - Boltzmann, Fermi Dirac & Bose-Einstein Statistics- comparison. Partition functions-evaluation of translational, vibrational and rotational partition functions for monoatomic, diatomic and polyatomic ideal gases. Thermodynamic functions in terms of partition functions calculation of equilibrium constants. Statistical approach to

Thermodynamic properties: pressure, internal energy, entropy, enthalpy, Gibb's function, Helmholtz function, residual entropy and equilibrium constants. Heat capacity of mono and diatomic gases-ortho and para hydrogen. Heat capacity of solids-Einstein and Debye models.

UNIT-III:

Irreversible Thermodynamics: Theories of conservation of mass and energy, entropy production in open systems by heat, matter and current flow, force and flux concepts. Onsager theory-validity and verification- Onsager reciprocal relationships. Electro kinetic and thermo mechanical effects-Application of irreversible thermodynamics to biological systems.

UNIT-IV:

Kinetics of Reactions: Theories of reaction rates -effect of temperature on reaction rates, collision theory of reaction rates, Unimolecular reactions -Lindeman and Christiansen hypothesis. Potential energy surfaces. Transition state theory-evaluation of thermodynamic parameters of activation-applications of ARRT to reactions between atoms and molecules. Factors determine the reaction rates in solution - primary salt effect and secondary salt effect, Homogeneous catalysis- acid- base catalysis-mechanism of acid base catalyzed reactions-Bronsted catalysis law, enzyme catalysis-Michelis- Menton catalysis.

UNIT-V:

Kinetics of complex and fast reactions: Kinetics of complex reactions, reversible reactions, consecutive reactions, parallel reactions, chain reactions. Chain reactions-chain length, kinetics of H2– Cl2 & H2–Br2 reactions (Thermal and Photochemical reactions) – Rice Herzfeld mechanism. Study of fast reactions-relaxation methods temperature and pressure jump methods, electric and magnetic field jump methods - stopped flow, flash photolysis methods and pulse radiolysis. Kinetics of polymerization-free radical, cationic, anionic polymerization - Polycondensation.

Recommended Text

1. J. Rajaram and J.C. Kuriacose, Thermodynamics for Students of Chemistry, 2nd edition, S.L.N.Chand and Co., Jalandhar, 1986.
2. I.M. Klotz and R.M. Rosenberg, Chemical thermodynamics, 6Th edition, W.A. BenjaminPublishers, California, 1972.
3. M.C. Gupta, Statistical Thermodynamics, New Age International, Pvt. Ltd., New Delhi, 1995.
4. K.J. Laidler, Chemical Kinetics, 3rd edition, Pearson, Reprint - 2013.
5. J. Rajaram and J.C. Kuriokose, Kinetics and Mechanisms of chemical transformation, M acmillan India Ltd, Reprint - 2011.

Reference Books

1. D.A. Mcqurrie And J.D. Simon, Physical Chemistry – A Molecular Approach, Viva Books Pvt. Ltd., New Delhi, 1999.
2. R.P. Rastogi and R.R. Misra, Classical Thermodynamics, Vikas Publishing, Pvt. Ltd., New Delhi, 1990.
3. S.H. Maron and J.B. Lando, Fundamentals of Physical Chemistry, Macmillan Publishers, New York, 1974
4. K.B. Ytsiimiriski, "Kinetic Methods of Analysis", Pergamom Press,1996.
5. Gurdeep Raj, Phase rule, Goel Publishing House, 2011.

Website and e-learning source

1. https://nptel.ac.in/courses/104/103/104103112/
2. https://bit.ly/3tL3GdN

ORGANIC CHEMISTRY PRACTICAL - II

Objectives of the course

- To understand the concept of quantitative estimation of organic compounds.
- To develop analytical skill in the estimation of organic compounds.
- To construct suitable experimental setup for the organic preparations involving two stages.
- To experiment different purification and drying techniques for the compound processing.

UNIT-I: Estimations:

a. Estimation of Phenol (bromination)
b. Estimation of Aniline (bromination)
c. Estimation of Ethyl methyl ketone (iodimetry)
d. Estimation of Glucose (redox)
e. Estimation of Ascorbic acid (iodimetry)
f. Estimation of Aromatic nitro groups (reduction)
g. Estimation of Glycine (acidimetry)
h. Estimation of Formalin (iodimetry)
i. Estimation of Acetyl group in ester (alkalimetry)

UNIT-II: Two stage preparations:

a. p-Bromoaniline from acetanilide
b. p-Nitroaniline from acetanilide
c. 1,3,5-Tribromobenzene from aniline
d. Benzilic acid from benzoin
e. m-Nitroaniline from nitrobenzene
f. m-Nitrobenzoic acid from methyl benzoate

Recommended Text

1. A.I. Vogel, Elementary Practical Organic Chemistry: Small Scale Preparations, Qualitative Organic Analysis, Quantitative Organic Analysis, Pearson Education, 2011.
2. F.G. Mann and B.C. Saunders, Practical Organic Chemistry, 4th edn, Pearson Education India, 2009.
3. K. Bansal Raj, Laboratory Manual of Organic Chemistry, New Age International, 2009.
4. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu, Basic Principles of Practical Chemistry, Sultan Chand & Sons, 2004.
5. V.K. Ahluwalia, and R. Aggarwal, Comprehensive Practical Organic Chemistry, Universities Press, 2004.

Reference Books

1. R.G. Engel, D.L. Pavia, G.M. Lampman and G.S. Kriz, A Microscale approach to Organic Laboratory, 5th edition, Paperback – International Edition, 2012.
2. P.B. Cranwell, L.M. Harwood and C.J. Moody, Experimental Organic Chemistry, 3rd edn, Wiley-Blackwell, 2017.
3. J. Leonard, B. Lygo and G. Procter, Advanced Practical Organic Chemistry, 3rd edn, CRC Press, 2013.

Website and e-learning source

1. https://ocw.mit.edu/courses/3-091-introduction-to-solid-statechemistry-fall-2018/video_galleries/lecture-videos/

INORGANIC CHEMISTRY PRACTICAL-I

Objectives of the course

- To learn the principles and methods of qualitative analysis of familiar and less familiar cations present in a mixture.
- To identify the methodology to analyze qualitatively a metal ion in the presence of another metal ion.
- To recall the principle and theory in preparing standard solutions.
- To train the students for improving their skill in estimating the amount of ion accurately present in the solution

UNIT-I: Analysis of mixture of cations:

Analysis of a mixture of four cations containing two common cations and two rare cations. Cations to be tested.

Group-I : W and Pb.

Group IA : Se, Te

Group-II : Mo, Cu, Bi and Cd.

Group-III : Ce, Th, Zr, V, Cr, and Ti.

Group-IV : Zn, Ni, Co and Mn.
Group-V : Ba and Sr.
Group-VI : Li.

UNIT-II: Complexometric Titration:

1. Estimation of zinc, nickel, magnesium, and calcium.
2. Estimation of mixture of metal ions-pH control, masking and demasking agents.
3. Determination of calcium and lead in a mixture (pH control).
4. Determination of manganese in the presence of iron.
5. Determination of nickel in the presence of iron.

Recommended Text

1. A.JeyaRajendran, Microanalytical Techniques in Chemistry: Inorganic Qualitative Analysis, United global publishers, 2021.
2. V. V. Ramanujam, Inorganic Semimicro Qualitative Analysis; 3rded., The National Publishing Company, Chennai, 1974.
3. Vogel's Text book of Inorganic Qualitative Analysis, 4thed., ELBS, London.
4. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney, Vogel's Textbook of Quantitative Chemical Analysis, Revised 5th edition, ELBS, 1989.
5. Douglas A. Skoog, Donald M. West, F. James Holler and Stanley R. Crouch, Fundamentals of Analytical Chemistry, 8th Edition, Brooks/Cole-Thomson Learning, USA, 2004.

Reference Books

1. G. Pass, and H. Sutcliffe, Practical Inorganic Chemistry; Chapman Hall, 1965.
2. W. G. Palmer, Experimental Inorganic Chemistry; Cambridge University Press, 1954.

MEDICINAL CHEMISTRY

Objectives of the course

- To introduce the mechanism of drug action and drug delivery system
- To learn various types of drugs and their mode of action.
- To learn drug design and drug synthesis.

UNIT-I:

Introduction to receptors: Introduction, targets, Agonist, antagonist, partial agonist. Receptors, Receptor types, Theories of Drug – receptor interaction, Drug synergism, Drug resistance, physicochemical factors influencing drug action.

UNIT-II:

Antibiotics: Introduction, Targets of antibiotics action, classification of antibiotics, enzyme-based mechanism of action, SAR of penicllins and tetracyclins, clinical application of penicillins, cephalosporin. Current trends in antibiotic therapy.

UNIT-III:

Antihypertensive agents and diuretics: Classification of cardiovascular agents, introduction to hypertension, etiology, types, classification of antihypertensive agents, Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol. Classification and mechanism of action of diuretics, Furosemide, Hydrochlorothiazide, Amiloride.

UNIT-IV: Antineoplastic Agents

Antineoplastic Agents: Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer - Introduction of carcinolytic antibiotics and mitotic inhibitors - Synthesis of mechlorethamine, cyclophosphamide, melphalan, and uracil - Recent development in cancer chemotherapy.

UNIT-V: Analgesics, Anti-inflammatory and Antidiabetic Drugs:

Introduction, Mechanism of inflammation, classification and mechanism of action and paracetamol, Ibuprofen, Diclofenac, naproxen, indomethacin, phenylbutazone and meperidine. Antidiabetic Agents: Introduction, Types of diabetics, Drugs used for the treatment, chemical classification, Mechanism of action, Treatment of diabetic mellitus. Chemistry of insulin, sulfonyl urea.

Recommended Text

1. Wilson and Gisvold's textbook of organic medicinal and pharmaceutical chemistry,
2. Wilson, Charles Owens: Beale, John Marlowe; Block, John H, Lipincott William, 12th edition, 2011.
3. Graham L. Patrick, An Introduction to Medicinal Chemistry, 5^{th} edition, Oxford University Press, 2013. Jayashree Ghosh, A text book of Pharmaceutical Chemistry, S. Chand and Co. Ltd, 1999, 1999 edn.
4. O. LeRoy, Natural and synthetic organic medicinal compounds, Ealemi, 1976.
5. S. Ashutosh Kar, Medicinal Chemistry, Wiley Eastern Limited, New Delhi, 1993, New edn.

Reference Books

1. Foye’s Princles of Medicinal Chemistry, Lipincott Williams, Seventh Edition, 2012

2. Burger's Medicinal Chemistry, Drug Discovery and Development, Donald J. Abraham, David P. Rotella, Alfred Burger, Academic press, 2010.
3. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, John M. Beale Jr and John M. Block, Wolters Kluwer, 2011, 12th edn.
4. P. Parimoo, A Textbook of Medical Chemistry, New Delhi: CBS Publishers.1995.
5. S. Ramakrishnan, K. G. Prasannan and R. Rajan, Textbook of Medical Biochemistry, Hyderabad: Orient Longman. 3rd edition, 2001.

Website and e-learning source

1. https://www.ncbi.nlm.nih.gov/books/NBK482447/
2. https://training.seer.cancer.gov/treatment/chemotherapy/types.html
3. https://www.classcentral.com/course/swayam-medicinal-chemistry6012908

GREEN CHEMISTRY

Objectives of the course

- To understand the basic principles of Green chemistry and Green techniques.
- To study Green catalysis and Green solvents.
- To propose solutions for pollution prevention in Industrial chemical and fuel production, Automotive industry and Shipping industries.
- To propose green solutions for industrial production of Organic and inorganic chemicals.

UNIT-I:

Basic Principles of Green Chemistry: Introduction- Need for Green Chemistry. Goals of Green Chemistry. Limitations of Green Chemistry. Chemical accidents, terminologies, International green chemistry organizations and Twelve principles of Green Chemistry with examples.

UNIT-II:

Green Synthesis: Choice of starting materials, reagents, catalysts and solvents in detail, Green chemistry in day today life. Designing green synthesis-Green reagents: dimethyl carbonate. Green solvents: Water, Ionic liquids - criteria, general methods of preparation, effect on organic reaction. Supercritical carbon dioxide- properties, advantages, drawbacks and a few examples of organic reactions in scCO2. Green synthesis-adipic acid and catechol.

UNIT-III:

Green Catalysis: Environmental pollution, Green Catalysis- Acid catalysts, Oxidation

catalysts, Basic catalysts, Polymer supported catalysts-Poly styrene aluminum chloride, polymeric super acid catalysts, Polymer supported photosensitizers.

UNIT-IV:

Greener Reactions: Phase transfer catalysis in green synthesis-oxidation using hydrogen peroxide, crown ethersesterification, saponification, anhydride formation, Elimination reaction, Displacement reaction. Applications in organic synthesis.

UNIT-V:

Green Techniques: Micro wave induced green synthesis - Introduction, Instrumentation, Principle and applications. Sonochemistry – Instrumentation, Cavitation theory - Ultra sound assisted green synthesis and Applications.

Recommended Text

1. Ahluwalia, V.K. and Kidwai, M.R. New Trends in Green Chemistry, Anamalaya Publishers, 2005.
2. W. L. McCabe, J.C. Smith and P. Harriott, Unit Operations of Chemical Engineering, 7thedition, McGraw-Hill, NewDelhi,2005.
3. J. M. Swan and D. St. C. Black, Organometallics in Organic Synthesis, Chapman Hall,1974.
4. V. K. Ahluwalia and R. Aggarwal, Organic Synthesis: Special Techniques, Narosa Publishing House, New Delhi,2001.
5. A.K. De, Environmental Chemistry, New Age Publications, 2017.

Reference Books

1. Anastas, P.T. and Warner, J.K. Oxford Green Chemistry -Theory and Practical, University Press, 1998
2. Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker, 2001
3. Cann, M.C. and Connely, M.E. Real-World Cases in Green Chemistry, American Chemical Society, Washington, 2000
4. Ryan, M.A. and Tinnesand, M., Introduction to Green Chemistry, American Chemical Society Washington, 2002.
5. Chandrakanta Bandyopadhyay, An Insight into Green Chemistry, Books and Allied (P) Ltd, 2019.

Website and e-learning source

1. https://www.organic-chemistry.org/
2. https://www.studyorgo.com/summary.php

BIO INORGANIC CHEMISTRY

Objectives of the course

- To understand the role of trace elements.
- To understand the biological significance of iron and sulphur.
- To study the toxicity of metals in medicines.
- To have knowledge on diagnostic agents.
- To discuss on various metalloenzymes properties.

UNIT-I:

Essential trace elements: Selective transport and storage of metal ions: Ferritin, Transferrin and siderophores; Sodium and potassium transport, Calcium signaling proteins. Metalloenzymes: Zinc enzymes–carboxypeptidase and carbonic anhydrase. Iron enzymes– catalase, peroxidase. Copper enzymes – superoxide dismutase, Plastocyanin, Ceruloplasmin, Tyrosinase. Coenzymes - Vitamin-B12 coenzymes.

UNIT-II:

Transport Proteins: Oxygen carriers - Hemoglobin and myoglobin - Structure and oxygenation Bohr Effect. Binding of CO, NO, CN– to Myoglobin and Hemoglobin. Biological redox system: Cytochromes-Classification, cytochrome a, b and c. Cytochrome P-450. Non-heme oxygen carriers-Hemerythrin and hemocyanin. Iron-sulphur proteins- Rubredoxin and Ferredoxin- Structure and classification.

UNIT-III:

Nitrogen fixation: Introduction, types of nitrogen fixing microorganisms. Nitrogenase enzyme - Metal clusters in nitrogenase- Transition metal complexes of dinitrogen - nitrogen fixation via nitride formation and reduction of dinitrogen to ammonia. Photosynthesis: photosystem-I and photosystem-II-chlorophylls structure and function.

UNIT-IV:

Metals in medicine: Metal Toxicity of Hg, Cd, Zn, Pb, As, Sb. Therapeutic Compounds: Vanadium-Based Diabetes Drugs; Platinum-Containing Anticancer Agents. Chelation therapy; Cancer treatment. Diagnostic Agents: Technetium Imaging Agents; Gadolinium MRI Imaging Agents.

UNIT-V:

Enzymes - Introduction and properties - nomenclature and classification. Enzyme kinetics, free energy of activation and the effects of catalysis. Michelis - Menton equation - Effect of pH, temperature on enzyme reactions. Factors contributing to the efficiency of enzyme.

Recommended Text

1. Williams,D.R. –Introdution to Bioinorganic chemistry.
2. F.M. Fiabre and D.R. Williams– The Principles of Bioinorganic Chemistry,RoyolSoceity of Chemistry, Monograph for Teachers-31
3. K.F. Purcell and Kotz., Inorganic chemistry, WB Saunders Co., USA.
4. G.N. Mugherjea and Arabinda Das, Elements of Bioinorganic Chemistry - 1993.
5. R. Gopalan, V. Ramalingam, Concise Coordination Chemistry, S. Chand, 2001.

Reference Books

1. M.Satake and Y.Mido, Bioinorganic Chemistry- Discovery Publishing House, New Delhi (1996)
2. M.N. Hughes, 1982, The Inorganic Chemistry of Biological processes, II Edition, Wiley London.
3. R.W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987.
4. R.M. Roat-Malone, Bio Inorganic Chemistry, John Wiley, 2002.
5. T.M. Loehr, Iron carriers and Iron proteins, VCH, 1989.

Website and e-learning source

1. https://www.pdfdrive.com/instant-notes-in-inorganic-chemistrythe-instant-notes-chemistry-series-d162097454.html
2. https://www.pdfdrive.com/shriver-and-atkins-inorganic-chemistry-5th-edition-d161563417.html

MATERIAL SCIENCE

Objectives of the course

- To understand the crystal structure, growth methods and X-ray scattering.
- To explain the optical, dielectric and diffusion properties of crystals.
- To recognize the basis of semiconductors, superconductivity materials and magnets.
- To learn about the importance of materials used for renewable energy conversion.

UNIT-I:

Crystallography: symmetry - unit cell and Miller indices - crystal systems - Bravais lattices - point groups and space groups – Xray diffraction-Laue equations-Bragg's law-reciprocal lattice and its application to geometrical crystallography. Crystal structure–powder and single crystal applications. Electron charge density maps, neutron diffraction-method and applications.

UNIT-II:

Crystal growth methods: Single crystal –Low and high temperature, solution growth– Gel and sol-gel. Crystal growth methodsnucleation– equilibrium stability and metastable state. Melt growth - Bridgeman-Stockbarger, Czochralski methods. Flux technique, physical and chemical vapour transport. Lorentz and polarization factor - primary and secondary extinctions. Characterization–TG/DTA/DSC methods, SEM/TEM Analysis. Determination of Hardness, Applications of Single Crystals.

UNIT-III:

Properties of crystals: Optical studies – Electromagnetic spectrum (qualitative) refractive index – reflectance – transparency, translucency and opacity. Types of luminescence – photo-, electro-, and injection luminescence, LEDs – organic, Inorganic and polymer LED materials - Applications. Dielectric studies- Polarisation - electronic, ionic, orientation, and space charge polarisation. Effect of temperature. dielectric constant, dielectric loss. Types of dielectric breakdown– intrinsic, thermal, discharge, electrochemical and defect breakdown.

UNIT-IV:

Special Materials: Superconductivity: Meissner effect, Critical temperature and critical magnetic Field, Type I and II superconductors, BCS theory-Cooper pair, Applications. Soft and hard magnets – Domain theory Hysteresis Loop-Applications. Magneto and giant magnetoresistance. Ferro, ferri and antiferromagnetic materials applications, magnetic parameters for recording applications. Ferro-, Piezo-, and pyro electric materials – properties and applications. Shape memory Alloys-characteristics and applications, Non-linear optics- Second Harmonic Generators, mixing of Laser wavelengths by quartz, ruby and LiNbO3.

UNIT-V:

Materials for Renewable Energy Conversion: Solar Cells: Organic, bilayer, bulk heterojunction, polymer, perovskite based. Solar energy conversion: lamellar solids and thin films, dye-sensitized photo voltaic cells, coordination compounds anchored to semiconductor surfaces - Ru(II) and Os(II) polypyridyl complexes. Photochemical activation and splitting of water, CO2 and N2. Manganese based photo systems for water-splitting. Complexes of Rh, Ru, Pd and Pt - photochemical generation of hydrogen from alcohol.

Recommended Text

1. S. Mohan and V. Arjunan, Principles of Materials Science, MJP Publishers, 2016.
2. Arumugam, Materials Science, Anuradha Publications, 2007.

3. Giacavazzo et. al., Fundamentals of Crystallography, International Union of Crystallography. Oxford Science Publications, 2010
4. Woolfson, An Introduction to Crystallography, Cambridge University Press, 2012.
5. James F. Shackelford and Madanapalli K. Muralidhara, Introduction to Materials Science for Engineers. 6th ed., PEARSON Press, 2007.

Reference Books

1. Suggested Readings 1. M.G. Arora, Solid State Chemistry, Anmol Publications, New Delhi, 2001.
2. R.K. Puri and V.K. Babbar, Solid State Physics, S Chand and Company Ltd, 2001.
3. Kittel, Solid State Physics, John-Wiley and sons, NY, 1966.
4. H.P. Meyers, Introductory Solid State Physics, Viva Books Private Limited, 1998.
5. A.R. West, Solid State Chemistry and Applications, John-Wiley and sons, 1987.

Website and e-learning source

1. http://xrayweb.chem.ou.edu/notes/symmetry.html.
2. http://www.uptti.ac.in/classroom-content/data/unit%20cell.pdf.
3. https://bit.ly/3QyVg2R

COMPUTATIONAL CHEMISTRY

Objectives of the course

- To understand the concept of Computational chemistry.
- To impart skills on use of various chemistry tools that are essential for any student with chemistry as a major course.
- To learn the techniques of molecular simulations which will enhance the students' employability in academia and industry.

UNIT- I:

Basics: Need of Computational Chemistry – Tools of Computational Chemistry: Molecular Mechanics – Force field – Principles of Molecular mechanics – Merits and Demerits. Ab initio calculations: Principles of ab initio method – Hartree fock equations – Merits and Demerits. Semi empirical calculations : Basic principles – PPP, CNDO, INDO and NDDO methods – Merits and Demerits. Density Functional calculations – Basic principles – Kohn-Sham approach – Merits and Demerits.

UNIT- II:

Applications of Computational Chemistry: – Geometry optimization – Vibrational frequency analysis – Dipole moment – Bond order – Charges: Mulliken, Natural and Hirshfeld Charges – UV and NMR spectra, Electronegativity, Hardness, Softness, Fukui function.

UNIT- III:

Molecular Docking: Online servers for the selection of macromolecules and ligands – RCSB – Chemdata base – Online servers to detect druglikeness of compound - Swiss ADME – Molinspiration – ADMET servers – Preparation of macromolecule and ligand – Autodock Vina – Binding energy – Types of interactions between macromolecule and ligand - Molecular interaction visualizing softwares – Discovery Studio.

UNIT- IV:

Computing software – I: Introduction and stepwise approach to Chemdraw, ACD/Chemsketch and Argus Lab.

Exercises:

1. Drawing the structures of organic molecules and reaction schemes using Chemdraw or ACD/Chemsketch.
2. Geometry optimization and single point energy calculations of simple organic molecules.
3. Calculation of dipole moment in polar organic molecules.

UNIT- V:

Computing Software – II: Introduction and stepwise approach to AVOGADRO, Molinspiration, SwissADME, SwissDock, and Autodock.

Exercises:

1. Calculation of molecular properties and bioactivity of the simple drug molecules like aspirin, paracetamol, and the drugs of your choices using the online server molinspiration.
2. Prediction of drug likeliness, ADME and Toxicity of the drug classes like antibiotics, antihistamines, anesthetics and drug molecules of your choice using online server SwissADME or SwissDock.
3. Perform molecular docking of your choice using Autodock tools or Autodock Vina or Argus Lab.

Recommended Text

1. Frank Jensen, Introduction to Computational Chemistry, Third Edition, John Wiley & Sons, 2017.
2. Andrew R. Leach, Molecular modelling: principles and applications, Second Edition, Prentice-Hall, 2001.
3. Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Models, Second Edition, John Wiley & Sons, 2004.

Reference Books

1. Jan H. Jensen, Molecular Modelling Basics, CRC Press, 2010.
2. Waren J. Hehre, Alan J. Shusterman and Janet E. Nelson, The molecular modelling workbook for organic chemistry, Wavefunction Inc., 1998.
3. James B. Foresman and Eleen Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., Third Edition, 2015.

Website and e-learning source

1. https://onlinecourses.nptel.ac.in/noc20_cy08/preview
2. https://www.digimat.in/nptel/courses/video/104106122/L14.html