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 2021-2022 onwards)

Semester-IV				
Part	**Subject Status**	**Subject Title**	**Subject Code**	**Credit**
3	Core	SYNTHETIC STRATEGIES IN ORGANIC CHEMISTRY	ZCHM41	4
3	Core	BIOINORGANIC, SPECTRAL METHODS-II AND PHOTOCHEMISTRY	ZCHM42	4
3	Core	CHEMICAL KINETICS, PHOTOCHEMISTRY AND SURFACE CHEMISTRY	ZCHM43	4
3	Core	SELECTED TOPICS IN CHEMISTRY	ZCHM44	4
3	Core Practical	COMPUTATIONAL SOFTWARE IN CHEMISTRY - LABORATORY COURSE	ZCHL41	2
3	Core	PROJECT	ZCHP41	6

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

SYNTHETIC STRATEGIES IN ORGANIC CHEMISTRY

Objectives:

- To study selected name reactions and synthetic utility of important organic reagents.
- To understand the concept of retrosynthesis and the terms involved, about one group and two group disconnections and protection and deprotection of important functional groups.
- To study about Steroids, Vitamins and Terpenoids.

UNIT I - NAME REACTIONS IN ORGANIC SYNTHESIS

Acyloin condensation, Shapiro reaction, Julia olefination, Bamford – Stevens reaction, Bouveault-Blanc Reduction, Oxymercuration, Mc Murray coupling, Mukaiyama aldol reaction, Hofmann-Loffler-Freytag reaction, Peterson olefination, Wittig reaction, Tischenko reaction, Ugi reaction, Nef reaction.

UNIT II - RETEROSYNTHETIC ANALYSIS

Disconnection approach - Synthon-synthetic equivalent, target molecule - Functional group interconversions – Chemoselectivity - one group C-C and C-X disconnection (disconnection of alcohols, alkenes, and carbonyl compounds) -Two group C-C & C-X disconnections: 1,3 and 1,5 difunctionalised compounds, α,β- unsaturated carbonyl compounds, synthesis of 3,4,5 and 6 membered rings in organic synthesis. Diels-Alder reaction, Robinson annulation reaction.

Use of protecting groups for alcohols, amines, acids, carbonyl compounds- use of activating and blocking groups – Reversal of polarity (Umpolung) - Reterosynthetic analysis of the following compounds: cis - Jasmone, Trihexyl phenydyl, Isonootkatone, cascarillic acid, and 2,4-dimethyl-2-hydroxy pentanoic acid.

UNIT III - REAGENTS IN ORGANIC SYNTHESIS

Uses of the following reagents in organic synthesis and functional group transformation:

2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), DMSO, Super hydrides - Dess-martin- periodinane.

Modern Reagents: Introductory treatment of the application of silicon (Tri alkyl silyl halides, organo silanes), Boron (9–BBN, borane, and alkyl borane), phosphorus (phosphoranes), Tin – allyl stannane, palladium (Stille coupling, Suzuki Coupling, Heck and Negishi reactions) samarium (SmI2), ruthenium (RuO4, Ru-BINAP Complex), platinum (Adam's Catalyst) reagents.

UNIT IV - STEROIDS

Classification- structural elucidation of cholesterol, irradiated products of ergosterol. Conversion of cholesterol to androsterone, progesterone, testosterone, 5α- and 5 β-cholanic acid. Conversion of Oestrone to Oestriol, Oestrodiol and vice-versa. Conformational structure of cholestane and Coprostane. General study of Bile acids and Prostoglandins.

UNIT V - VITAMINS AND TERPENOIDS

Vitamins: Structural elucidation, synthesis of vitamins – A1, B1 and C - synthesis of vitamins B2, B6, D and E.

Terpenoids: Structural elucidation, synthesis of α-Pinene, Camphor, α-Cadinene, Zingiberene and squalene - synthesis of α-Santonin and Gibberelic acid.

PRESCRIBED BOOKS

1. B. P. Mundy, M. G. Ellerd, & F. G. Favaloro. Name Reactions and Reagents in Organic Synthesis, Wiley-Interscience, 2005.
2. A. Hassner and I. Namboothiri, Organic Syntheses Based Name Reactions, Elsevier , 2012.
3. W. Carruthers, and I. Coldham, Modern Methods of Organic Synthesis, Fourth edition, Cambridge University Press, 2015.
4. Dr Jagdamba Singh and Dr. L.D.S Yadav, Orgnic Synthesis: Design, Reagents, Reactions and Rearrngements, A Pragati Second Revised Edition, 2007.
5. E. J. Corey & X. M. Cheng, The Logic of Chemical Synthesis, Wiley-India Private Ltd, 2011.
6. S. Warren & P. Wyatt, Organic Synthesis: The Disconnection Approach, John Wiley & Sons, 2008.
7. Sanyal and Sanyal, Reactions, Rearrangements and Reagents, Fourth edition, Bharati Bhawan Publishers and Distributors, 2003.
8. N.R. Krishnaswamy, Chemistry of Natural Products; A Unified Approach, CRC Press; 2nd edition, 2010.
9. I.L. Finar, Organic Chemistry, Vol II, 5th edition, Pearson Education India, 2002.

REFERENCE BOOKS

1. L. Kurti & B. Czako, Strategic Applications of Named Reactions in Organic Synthesis, Elsevier 2005.
2. Jie Jack Li, Name Reactions, Fifth edition (Springer), 2014.
3. Thomas Laue and Andreas Plagens, Named Organic Reactions, John Wiley & Sons, 1999.

4. F. A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th edition, Springer, 2007.
5. R. O.C. Norman and J. M. Coxon, Principles of Organic Synthesis, 3rd edition, 1993.
6. P. Wyatt & S. Warren, Organic Synthesis: Strategy and Control, Wiley-Blackwell, 2007.
7. S. Warren, Designing Organic Synthesis, John Wiley & Sons, 1994.
8. D. Goldsmith, M. C. Pirrung and A. T. Morehead, Total Synthesis of Natural Products, John Wiley & Sons, 2007.
9. R. Xu, Y. Ye and W. Zhao, Introduction to Natural Products Chemistry, CRC Press, 2011.
10. D. Barton, K. Nakanishi and O. Meth-Cohn, Comprehensive Natural Products Chemistry, Elsevier 1999.
11. D. L. Nelson and M. M. Cox, Lehninger's Principles of Biochemistry, Seventh edition, WH Freeman, 2017.
12. J.M. Berg, J.L. Tymoczko and L. Stryer, Biochemistry, Fifth edition, W.H.Freeman and Co Ltd, 2002.

BIOINORGANIC, SPECTRAL METHODS-II AND PHOTOCHEMISTRY

Objectives:

- To introduce bioinorganic chemistry and to study role of metalloporphrins and metalloenzymes in various biological processes.
- To study the applications of Mossbauer and nuclear quadrupole resonance spectroscopic techniques in inorganic systems.
- To study the applications of NMR and EPR techniques in inorganic systems.
- To introduce inorganic photochemistry and to study applications in various systems.

UNIT I - BIOINORGANIC CHEMISTRY– I

Biological function, toxicity and deficiency of trace elements (N, O, F, Na, Mg, P, S, K, Ca, Cr, Mn, Fe, Co, Cu, Zn, As, Mo, Cd, Hg, I, Pb); classification of metallo-biomolecules. Metalloporphyrins – chlorophyll and photosynthesis; cytochromes, hemoglobin, myoglobin and dioxygen binding, vitamin B12 and co-enzyme – in vivo and in vitro nitrogen fixation. Iron storage and transport: ferritin, transferrins and siderophores, iron proteins: hemerythrin, cytochrome P450 enzyme, ferredoxin and rubredoxin.

UNIT II - BIOINORGANIC CHEMISTRY– II

Copper proteins and Enzymes:peroxidases,catalases,oxygenases, plastocyanin, azurin, hemocyanin and ascorbic oxidase – different types of Cu present in proteins and enzymes. Zinc enzymes: carboxypeptidase A, carbonic anhydrase and superoxide dismutase. Inhibition and poisoning of enzymes illustrated by xanthine oxidase and aldehyde oxidase. Chelate therapy – metal complexes as drugs, anticancer and antiarthritic agents. Metal complexes as probes of nucleic acids.

UNIT III - MOSSBAUER SPECTROSCOPY

Splitting of resonance lines: quadrupole splitting and magnetic hyperfine splitting. Applications: MB spectra of iron compounds/complexes – structural elucidation, π-bonding effect, determination of high spin and low spin, spin state crossover and cis–trans isomers – nature of the complexes – mixed valence complexes. Tin compounds: MB spectra of Sn(II) and Sn(IV) compounds, oxidation states of Sn in its different compounds. Applications in bioinorganic chemistry: oxy and deoxy- hemerythrin - catalase, peroxidases, Fe-S protein systems.

UNIT IV - NMR AND ESR SPECTROSCOPY

NMR Spectroscopy: ^{1}H, ^{19}F and ^{31}P – NMR – applications in structural problems based on number of signals, multiplicity, anisotropy (like H_3PO_3, H_3PO_2, $[HN_i(PPh_3)_4]+$, SF_4, TiF_4, PF_5, HPF_2, H_2PF_3, $PF_3(NH_2)_2$, P_4S_3, $P_4N_4Cl_6(NHC_6H_5)_2$, $P_3N_3(CH_3)_2Cl_4$, NF_3, NH_3 – mer- and fac-$Rh(PPh_3)_3Cl_3$. B^{11} NMR of B_3H_8- and $B_{10}H_{14}$. Fluxional molecules (including organometallic compounds) and study of fluxionality by NMR technique - NMR of paramagnetic molecules - contact shifts. Evaluation of Rate constants - monitoring the course of reaction using NMR.

EPR spectroscopy: Hyperfine splitting - Factors affecting magnitude of g-values - Zero field splitting and Kramers' degeneracy - Application of EPR in the study of transition metal complexes based on number of signals, multiplicity, anisotropy (bis(salicylaldimine)copper(II), $[Cu(bpy)_3]^{2+}$, $[Cu(Phen)Cl_2]$, $[(NH_3)_5Co\text{-}O_2\text{-}Co(NH_3)_5]^{5+}$ $Co_3(CO)_9Se$, $Co_3(CO)_9Rh$, $[CoF_6]^{4-}$, $[CrF_6]^{3-}$, $VO(acac)_2$, $[VO(H_2O)_6]^{2+}$, $[Fe(CN)_5NO]^{2-}$, Applications in predicting the covalent character of M-L bond and Jahn-Teller distortion in Cu(II) complexes. EPR spectroscopy of metallobiomolecules: copper and iron proteins.

UNIT V - PHOTOCHEMISTRY OF METAL COMPLEXES

Properties of excited states of metal complexes – types of excited states, Frank Condon and thermally equilibrated excited (THEXI) states – photophysical processes: bimolecular deactivation and energy transfer, photochemical processes: electron transfer reactions, isomerisation and substitutional processes – Photochemistry of Cr(III) and Co(III) complexes - Photophysical and photochemical properties of

$[Ru(bpy)_3]^{2+}$ and $[Cr(bpy)_3]^{3+}$. Applications of inorganic photochemistry: photochemical conversion and storage of solar energy – photochemical conversion of N_2 to NH_3 – TiO_2 as a green photocatalyst in removing air and water pollutants.

PRESCRIBED BOOKS

1. James E. Huheey, Ellen A. Keiter and Richard L. Keiter, Inorganic chemistry: principles Structure and Reactivity, 4th Edition, Pearson Education, 2006.
2. P. Atkins, T. Overton, J. Rourke, M. Weller and F.Armstrong, Inorganic Chemistry, 5th edition, Oxford University press, 2010.
3. Russell S. Drago, Physical Methods in Inorganic Chemistry, Chapman and Hall Ltd., London, 1965.
4. Russell S. Drago, Physical Methods for Chemists, Surfside Scientific Publishers, 2nd Edition, 1977.
5. E.A.V. Ebsworth, David W.H. Rankin and Stephen Credock, Structural Methods in Inorganic Chemistry, ELBS, 1988.
6. I.Bertini, H.B.Gray, S.J.Lippard and J.S.Valantine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., 1998.
7. S.J.Lippard and J.M.Berg, Principles of Bioinorganic Chemistry, Panima Company, New Delhi, 1997.
8. K.K. Rohatgi – Mukherjee, Fundamentals of Photochemistry, Wiley, New York, 3rd Edition, 2002.
9. D.E. Fenton, Bio-coordination Chemistry, Oxford Science Publications, 1995.

REFERENCE BOOKS

1. F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Marilo and Manfred Bochman, Advanced Inorganic Chemistry, Wiley Interscience Publication, 6th Edition, 2008.
2. David W. H. Rankin, Norbert W. Mitzel and Carole A. Morrison, Structural Methods in Molecular Inorganic Chemistry, John Wiley & Sons, Ltd, 1st Edition, 2013.
3. John A. Weil and James R. Bolton, Electron Paramagnetic Resonance Elementary Theory and Practical Applications, 2nd Edition, John Wiley & Sons, 2007.
4. E.I. Solomon and A.B.P. Lever, Inorganic Electronic Structure and Spectroscopy, Vol. 2 , Applications and case studies , Wiley – Interscience, 2006.
5. R.V. Parish, NMR, NQR, EPR and MOSSBAUER Spectroscopy in Inorganic Chemistry, Ellis Horwood Limited, 1990.
6. A.W. Adamson and P.D. Fleischauer, Concepts of Inorganic Photochemistry, John wiley and sons, New York, 1975.
7. K. Kalyanasundaram, Photochemistry of polypyridine and phorphyrin

complexes, Academic Press, London, 1992.

CHEMICAL KINETICS, PHOTOCHEMISTRY AND SURFACE CHEMISTRY

Objectives:

- To educate the kinetic theory of gases.
- To explain various concepts of Phase rule.
- To elucidate the use of chemical kinetics in understanding reaction mechanisms and to apply the theories and concepts of it for homogenous and heterogeneous catalyzed reactions.
- To understand the photochemical organic reactions and radiation chemistry reactions.
- To understand the surface phenomena.

UNIT I - KINETIC THEORY OF GASES AND PHASE RULE

Equations of state - molecular speeds - distribution of molecular velocities - one, two and three dimensions (Maxwell distribution of molecular velocity) - Maxwell distribution as energy distribution - Maxwell Boltzmann distribution law - Principle of equipartition energy and quantization - calculation of vibrational heat capacity - transport properties - thermal conductivity in a gas - the molecular collisions and mean free path in a gas - viscosity - diffusion of gases - nonsteady state - Poiseuille formula.

Phase rule and Lever rule - Derivation of phase rule from the concept of chemical potential. Plots for a mixture of three liquids consisting of one, two and three pairs of partially miscible liquids. Salting out phenomenon - systems composed of two solids and a liquid.

UNIT II - CHEMICAL KINETICS –I

Simple collision theory, absolute reaction rate theory, thermodynamics treatment, potential Energy surfaces, application of ARRT to simple bimolecular processes - steady state approximation, principle of microscopic reversibility & detailed balancing - chain reactions - general characteristics, study of kinetics of chain reactions like decomposition of acetaldehyde and N_2O_4; study of H_2-O_2 explosive reactions. Reactions in solutions - Factors determining reaction rates in solution; primary and secondary salt effects - influence of ionic strength and dielectric constant on reactions involving (i) ions (ii) dipoles (iii) ion and dipole. Electrostriction; influence of hydrostatic pressure; volume of activation. Linear free energy relationship, Hammett and Taft equations.

UNIT III - CHEMICAL KINETICS – II

Theory of unimolecular reactions - Lindemann, Hinshelwood, RRK, RRKM and Slater treatments. General catalytic mechanisms. Equilibrium and steady state treatments. Enzyme catalysis, Michalis-Menten kinetics, activation energies of enzyme-catalyzed reaction. Acid - base catalysis - protolytic and prototropic mechanisms. Acidity functions - Kinetic methods of analysis. Fast reaction techniques - Relaxation theory and relaxation techniques - Temperature, Pressure, electric field and magnetic field jump methods; Flash photolysis and pulse radiolysis, ultrasonic absorption techniques, reaction in a flow system, continuous and stopped flow, shock wave tube method.

UNIT IV - PHOTOCHEMISTRY AND RADIATION CHEMISTRY

Physical properties of the electronically excited molecules - excited state dipole moments, excited state pKa, excited state redox potential. Fluorescence, phosphorescence and other deactivation process - Stern-Volmer equation and its applications. Photosensitisation and chemiluminescence. Experimental techniques in photochemistry - flash photolysis technique. Radiation chemistry - source of high energy - interaction of high energy radiation with matter, radiolysis of water - definition of G value. Primary and secondary process, linear energy transfer - the hydrated electron and its reactions.

UNIT V - SURFACE CHEMISTRY AND CATALYSIS

Micelles - surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration(CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization - reverse micelles. Chemisorption and Physisorption; Langmuir's adsorption isotherm; competitive adsorption - Mechanisms of reactions on surfaces (Langmuir, Rideal and Langmuir-Hinshelwood mechanisms) Activation energies - Non-ideal adsorption; multiplayer adsorption; capillary condensation; measurement of surface area, BET equation , Gibbs adsorption isotherm - electrokinetic phenomena - zeta potential - Catalysis and types of catalysis - Heterogeneous catalysis - reactions and their kinetics.

PRESCRIBED BOOKS

1. J. Rajaram and J.C. Kuriokose, Kinetics and Mechanisms of chemical transformation, 1stEdn., Macmillan India Ltd., Delhi, 1993.
2. C. Kalidas, Chemical Kinetics methods, New-Age International, 1996.
3. K.J. Laidler, ChemicalKinetics, 3rdedn., Harper and Row Publishers, New York, 1987.
4. A.A. Frost and R.G. Pearson, Kinetics and Mechanism, 2nd edn., John Wiley and sons INC., 1963.
5. D.K. Chakrabarty and B. Viswanathan, Heterogeneous Catalysis, New Age Science Ltd, 2008.

REFERENCE BOOKS

1. Walter J. Moore, Physical Chemistry, 5th edition, Orient Longman, 1976.
2. G.W. Castellan, Physical Chemistry, 3rd edition, Addision-Weslay, 1986.
3. P. Atkins, Physical Chemistry, 7th edition, Oxford University Press, 2000.
4. K.B. Ytsiimiriski, Kinetic Methods of Analysis, Pergamom press, 1993.
5. W. Adamson and A.P. Gast, Physical chemistry of surfaces, 6th Edn.,Wiley, 1997.
6. J.J. Bikerman, Surface Chemistry: Theory and Applications, 2nd Edition, Academic Press, 2013.

SELECTED TOPICS IN CHEMISTRY

Objectives:

- To understand the concept of Computational chemistry.
- To learn principle of corrosion, corrosion inhibition and separation techniques.
- To study Chemical sensors, Biosensors and Contrasting agents in medical diagnosis.

UNIT I - COMPUTATIONAL CHEMISTRY

Introduction to computational chemistry - quantum mechanics - schrodinger equation. Types of calculations – single point energy, geometry optimization, frequency prediction - Brief introduction of computational methods - Ab initio method, semi-empirical method, Density Functional Theory method, Molecular mechanics. Basis Sets - minimal basis sets, split valence basis sets, polarized basis sets, Diffuse functions, High angular momentum basis sets.

UNIT II - CORROSION SCIENCE

Principles of Corrosion – Definition – Types of Corrosion - Electro chemical principles of Corrosion – Corrosion monitoring methods - Coupon (weight

loss) – electrical resistance – gasometric – Potentiodynamic polarisation – impedance – hydrogen permeation – Corrosion inhibition – definition – Classification of inhibitors based on electrode process – mechanism of inhibitor action in acidic medium

UNIT III - SEPARATION TECHNIQUES

Solvent extraction - Methods of extraction and applications of solvent extraction, solid-phase extraction, micro extraction (SPME), solid-phase nano extraction (SPNE). Chromatography - thin layer chromatography, ion exchange chromatography and size exclusion chromatography – HPLC-outline study of instrument modules. Gas chromatography – basic instrumental set up-carriers, columns and detectors.

UNIT IV - SENSORS

Definitions for sensors and biosensors - Technical definitions: calibration, selectivity, sensitivity, reproducibility, detection limits, response time; Introduction to Transducers - primary and secondary types, Active and passive, Analog and Digital transducers.

Sensors based on sensing layer - Chemical sensor - semi-conductor gas sensors, solid electrolyte gas sensors, ion-selective electrode sensors, humidity sensors and field effecttransistor sensors. Bio-sensors - Enzymes based, Affinity-based biosensors, Inhibition-based biosensors; Cell-based biosensors (Membrane receptors and transporters).

UNIT V - CONTRASTING AGENTS IN MEDICAL DIAGNOSIS

MRI imaging: Principles of MRI - development of MRI contrasting agents - types of contrasting agents – Gadolinium based contrasting agents, Manganese based contrast agents - Advantages and disadvantages - Fe(III) and Fe(II) based contrast agents - merits and demerits. Routes of administration - Targeted and organ specific contrast agents.

Radio isotopic Imaging agents: principle, functions and requirements of radio isotopic imaging agents - types of nuclear imaging - PET, SPEC and CAT imaging - nuclear imaging agents –18F, 99mTc.

PRESCRIBED BOOKS

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. Edward Mc Cafferty, Introduction to Corrosion Science, First Edition, Springer, 2010.

4. D. Kealey and P.J. Haines, Instant Notes Analytical chemistry, First Edition, BIOS, 2002.
5. R. Gopalan, P. S. Subramanian and K. Rengarajan, Elements of Analytical Chemistry, Sultan Chand and Sons, New Delhi, 2005.
6. S. M. Khopkar, Basic concepts of analytical chemistry, Third edition, New age international, 2008.
7. G.R. Chatwal and S.K. Anand, Instrumental Method of Chemical Analysis, Himalaya Publishing house, fifth (Reprint), 2016.
8. Jiri Janata, Principle of Chemical Sensors, First edition, Springer Science, 1989.
9. Editor-Maartin Braddock, Biomedical Imaging: The Chemistry of Labels, Probes and Contrast Agents, Royal Society of Chemistry, 2012.

REFERENCE BOOKS

1. Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Models, Second Edition, John Wiley & Sons Ltd, 2004.
2. James B. Foresman, Exploring Chemistry with Electronic Structure Methods, Second Edition, Gaussian Inc, 1996.
3. R Winston Revie and Herbert Henry Uhlig, Corrosion and its Control, Fourth Edition, John Wiley & Sons, 2018.
4. Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, Fundamentals of Analytical Chemistry, Ninth edition, Brooks/Cole, 2013.
5. Brian R. Eggins, Chemical Sensors and Biosensors, First Edition, John Wiley & Sons Ltd, 2002.
6. Peter Grundler, Chemical Sensors, Springer, 2007.
7. Florinel-Gabriel Banica, Chemical Sensors and Biosensors-Fundamentals and applications, First Edition, John-Wiley &Sons, 2012.
8. Ursula E. Spichiger-Keller, Chemical Sensors and Biosensors for Medical and Biological Applications, Wiley-VCH, 1998.
9. Richard C. Dorf, Sensors, Nanoscience, Biomedical Engineering, and Instruments: Sensors Nanoscience Biomedical Engineering, CRC Press, 2006.
10. M.J. Usher and D.A. Keating, Sensors and Transducers, Second Edition, Macmillan Press Ltd, 1996.
11. Editors-Andre Merbach, Lother Helm and Eva Toth, The chemistry of Contrasting Agents in Medical Magnetic Resonance Imaging, Second Edition, John Wiley and Sons Ltd, 2013.
12. Editors-Valerie C. Pierre and Matthew J. Allen, Contrast Agents for MRI, Royal Society of Chemistry, 2018.

COMPUTATIONAL SOFTWARE IN CHEMISTRY LABORATORY COURSE

Objectives:

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

UNIT I - BASICS

Basic idea of Molecular Modelling – A brief introduction about computational methods and their applications in chemistry – Basic terminologies used in computational methods (relevant to the exercises given in UNIT II). Computing software - introduction and stepwise approach to Chemdraw, ACD/Chemsketch, Argus Lab, AVOGADRO, Molinspiration, preADMET, SwissADME, SwissDock, 1 – Click online server, Autodock, and Crystal Explorer.

Lectures include entire process of downloading and installation of the software.

UNIT II - HANDS ON EXERCISES

The experiments are related to the topics covered in B.Sc - M.Sc Chemistry courses. The students must do the following exercises depending on the availability of time and suitable computational chemistry software.

A. Drawing the structures of organic molecules and reaction schemes using Chemdraw or ACD/Chemsketch.

B. For the following experiments, Argus Lab or ACD/Chemsketch or Avogadro Molecular Editor or Gaussian software can be used. Minimum of six experiments is required to be carried out in this section.

    1. Geometry optimization and single point energy calculations of simple organic molecules.
    2. Calculation of energy gap between HOMO and LUMO in simple molecules and visualization of molecular orbitals.
    3. Calculation of dipole moment in polar organic molecules.
    4. Calculation of electrostatic charges of atoms in organic molecules using population analysis.
    5. Calculation of Resonance energy of aromatic compounds.
    6. Prediction of the stability of ortho, meta, para products of nitration of aromatic ring using computational chemistry calculations.
    7. Calculation of IR stretching frequencies of groups and visualization of normal modes of vibration in organic molecules.
    8. Calculation of dimerization energy of carboxylic acids.

9. Perform the conformational analysis of butane using potential energy scan.
10. Find the transition state of simple organic reactions and plot the reaction profile.
11. Determination of heat of hydration of organic molecules.
12. Find the Gibbs free energy of simple gaseous phase reactions and calculate equilibrium constant.
13. Spectral analysis (UV, IR and NMR) of simple organic molecules.
14. Calculation of pKa of simple organic molecules and compare it with experimental values.
15. Calculation of electrophilicity index in hard-soft acids and bases.

C. Prediction of molecular properties, bioactivity and molecular docking of drug molecules.

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 servers preADMET or SwissADME or SwissDock.
3. Perform molecular docking of your choice using 1-click docking online server tool at mcule.com. Website: https://mcule.com/ . First register at the site and perform molecular docking. Similarly, Autodock tools or Autodock Vina or Argus Lab can be used for molecular docking.

D. Learn to generate Hirshfeld surfaces, study the interaction energies and draw the electrostatic potential map using Crystal Explorer Software.

LINKS TO DOWNLOAD SOFTWARE

ACD/Chemsketch: https://www.acdlabs.com/resources/freeware/chemsketch/index.php
Molinspiration : https://www.molinspiration.com/
PreADMET : https://preadmet.bmdrc.kr/
SwissADME : http://www.swissadme.ch/index.php
Crystal Explorer: https://crystalexplorer.scb.uwa.edu.au/
1-click docking online server: https://mcule.com/
Autodock Tools Link: http://mgltools.scripps.edu/downloads
Autodock Vina Link: http://vina.scripps.edu/
Discovery Studio Visualizer: https://www.3dsbiovia.com/products/co..
Avogadro Molecular Editor : https://avogadro.cc/
ArgusLab : http://www.arguslab.com/arguslab.com/ArgusLab.html

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., Second Edition, 1996.
4. James B. Foresman and Eleen Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., Third Edition, 2015.
5. Donald W. Rogers, Heats of Hydrogenation: Experimental and Computational Hydrogen Thermochemistry of Organic compounds, World scientific Publishing Co, 2006.

PROJECT

Objectives:

- This course is designed to reinforce the concepts with analytical techniques.
- It provides a platform for students to have a hands-on experience with instruments and present a project report on a research topic.

Students will do the project work on a title approved by the respective project supervisor. Students will maintain daily records and present oral reports while doing the project. All the above process will be duly assessed by the project supervisor. They will submit the project report at the end of the semester.