DEPARTMENT OF CHEMISTRY

School of Physical Sciences

Central University of Kerala

Tejaswini Hills, Periye P.O.
Kasaragod 671320, Kerala

MSc Chemistry Syllabus

CURRICULUM & SYLLABUS OF M.Sc. CHEMISTRY

(Revised vide Board of Studies Meeting dated 29th January 2021 through email)

Programme outcome

- M.Sc chemistry at Central University of Kerala (CUK) will assure basic and advanced knowledge in all branches of chemistry like Physical, Organic, Inorganic, Analytical, etc.
- Students are provided special training in handling advanced instrumentation such as AAS, TGA, CHNS, GC, and spectrophotometric techniques.
- The choice of electives during the course is fully flexible; students can choose electives from any department as per their interest to streamline themselves towards an appropriate career.
- The course syllabus is constructed such that students can efficiently prepare for competitive exams and advanced research.

Specific outcome

- Career-based electives like instrumental methods of analysis, pharmaceutical chemistry, industrial catalysis, etc., are included in the syllabus.
- The practice of industrial visit to motivate students to take up their career in chemical industry and multinational companies.
- Prepare the students for writing manuscripts based on the research output from their M.Sc. dissertation work.

Participatory learning

- Many workshops, seminars, and conferences are conducted to motivate the M.Sc. students to present their M.Sc. dissertation work and acquire knowledge on current research activities in various topical areas.
- Students are also encouraged to participate in various academic activities.

Experimental learning

- M.Sc chemistry @CUK has a special mission on training students to handle scientific equipment; the practical course is formulated to have training on instrumentation techniques.

Skill development

- Students have to take up their dissertation work through which they will be trained to take up research problems and solve them.
- Through the project work they can acquire the basic and essential knowledge to take up research as a career.

- Also training acquired on handling instrument/scientific equipments make them suitable for any industrial job

Value added course

- All the core course syllabi are framed to enrich the students for attempting competitive exams.
- Elective courses are provided to enhance students' awareness of the current job opportunities and motivate them to do high-quality research.

M. Sc. CHEMISTRY

Structure and Scheme of Examination

Course Code	Course Title	Contact hrs. / wk.				Credits
		Lect	Lab	Tut	Total	
Semester I						
CHE 5101	Inorganic and Solid State Chemistry	4		1		4
CHE 5102	Organic Structure, Reactivity and Mechanism	4		1		4
CHE 5103	Symmetry and Group Theory	4		1		4
CHE 5104	Quantum Chemistry	4		1		4
CHE 5191	Inorganic Chemistry Laboratory- I		5			2
CHE 5192	Organic Chemistry Laboratory - I		5			2
	Total for Sem I	**16**	**10**	**4**	**30**	**20**
Semester II						
CHE 5201	Coordination Chemistry	4		1		4
CHE 5202	Organic Reactions and Synthesis	4		1		4
CHE 5203	Thermodynamics, Kinetic Theory & Statistical Mechanics	4		1		4
CHE 5204	Molecular Spectroscopy	4		1		4
CHE 5291	Physical Chemistry Laboratory - I		5			2
CHE 5292	Organic Chemistry Laboratory -II		5			2
	Total for Semester II	**16**	**10**	**4**	**30**	**20**
Semester III						
CHE 5301	Organo-metallic and Bio-inorganic Chemistry	4		1		4
CHE 5302	Organic Spectroscopy and Bio-organic Chemistry	4		1		4
CHE 5303	Reaction dynamics, Surface- & Electro-chemistry	4		1		4
Elective-I	*Anyone from the list approved by the Department/from the sister Department*	3		1		3
CHE 5391	Inorganic Chemistry Laboratory - II		5			2
CHE 5392	Physical Chemistry Laboratory - II		5			2
	Seminar			1		
	Total for Semester III	**15**	**10**	**5**	**30**	**19**
Semester IV						
Elective-II	*Anyone from the list approved by the Department/from the sister Department*	*3*		*1*		*3*
Elective III	*Anyone from the list approved by the Department/from the sister Department*	*3*		*1*		*3*
Elective IV	*Anyone from the list approved by the Department/from the sister Department*	*3*		*1*		*3*
CHE 5490	Dissertation / Project work			16		4
	Seminar			2		
	Total for Semester-IV	**9**		**21**	**30**	**13**
	Credits for Core Courses – all Semesters					**60**

	Credits for Elective Courses – all Semesters					**12**
	***ELECTIVE COURSES (Any four of the Department Electives OR Electives offered by other Departments within the University)**					
CHE 5001	Instrumental Methods of Analysis	3				3
CHE 5002	Chemistry of Biopolymers & Biochemical Reactions	3				3
CHE 5003	Computational Chemistry	3				3
CHE 5004	Electro-analytical Techniques	3				3
CHE 5005	Green Chemistry	3				3
CHE 5006	Industrial Catalysis	3				3
CHE 5007	Inorganic Photochemistry	3				3
CHE 5008	Materials Chemistry	3				3
CHE 5009	Nano Chemistry	3				3
CHE 5010	Natural Products Chemistry	3				3
CHE 5011	Polymer Chemistry	3				3
CHE 5012	Supramolecular Chemistry	3				3
CHE 5013	Renewable Energy	3				3
CHE 5014	Crystallography	3				3
CHE5015	Pharmaceutical Chemistry	3				3
CHE5016	Molecular Fluorescence and Applications	3				3
CHE5017	Physical Principles of Chemical Engineering	3				3
	Any one elective student may opted from Swayam platform (as mentioned below)					

***Elective Courses as well as their contents/scope may be added, deleted or revised anytime in accordance with the availability of facilities/faculty in the Department.**

*** The Department shall have the freedom to add, delete or revise the Elective Courses as well as their contents/scope at any time to match the availability of facilities/faculty.**

<u>Note 1:</u>

To provide an exposure for the students to R & D activities /industrial processes, it was felt necessary that they should visit National laboratories / Industrial establishments during the third or fourth semesters. A report on the visit shall be submitted by each student to the Head of the Department.

Details about the BOS recommended MOOC courses for the academic year July 2020 are as follows

Sl. No.	Course Name	Course Coordinator	Institute	Duration of the Course (weeks)	Credits
1.	Environmental Chemistry	Prof. AK Bhakshi	Delhi University	15	4
2.	Forensic Chemistry and Explosives	Prof. AK Gupta	SHIATS, Allahabad	15	4
3.	Bioorganic & Biophysical Chemistry	Prof. AK Bhakshi	Delhi University	15	4
4.	Research Ethics	Mr. Manoj Kumar K	INFLIBNET Centre, Gujarat	15	4
5.	Research Methodology	Prof. Bajpai	National Law University	15	4
6.	Academic Writing	Dr. Ajay Semalty	HNB Garhwal University	15	4
7.	Biomass Characterization	Prof. A. Arunkumar	Central University of Kerala	15	4
8.	Biophysical Chemistry	Prof. Pramit Kumar Chowdhury,	IIT-Delhi	12	3
9.	Laser: Fundamentals & Applications	Prof. Manbendra Chandra	IIT-Kanpur	8	2
10.	One and two dimensional NMR spectroscopy for chemistry	Prof. N. Suryaprakash	IISc Bangalore	12	3

Semester I

CHE 5101 Inorganic and Solid State Chemistry

Inorganic chains, rings, cages, and clusters,sulphur nitrogen compounds, polymeric sulphur nitride; isopoly anions, heteropoly anions; borazines; phosphonitrilic compounds, metal clusters, silicates, intercalcation chemistry, one dimensional conductors.

Boron cage compounds,boron hydrides, structure and bonding, styx numbers, the importance of icosahedral frame work of boron atoms in boron chemistry, closo, nido and arachno structure; carboranes, metallocene carboranes.

The lanthanides and actinides: Stable oxidation states, the lanthanide and actinide contractions; the f-orbitals, spectral and magnetic properties - comparison of inner transition and transition metals; separation of lanthanides; use of lanthanide compounds as shift reagents. Trans-actinide elements. Current applications of lanthanide compounds.

Nuclear structure; mass and charge, nuclear moments, binding energy, semi empirical mass equation, stability rules, magic numbers and models of nucleus. Equations of radioactive decay and growth, half-life, average life radioactive equilibrium–transient and secular equilibrium, determination of half-lives. Nuclear reactions, energetics of nuclear reactions, hot atom Chemistry, nuclear fission and fusion reactors.

The interaction of nuclear radiations with matter, Radiation hazards and therapeutics. Detectors and their principles.

Band theory of solids-energy bands, conductors and non-conductors, intrinsic semiconductors, extrinsic semiconductors, Hall effect.

Electrical properties; conductivity in pure metals; superconductivity; basics, discovery and high Tc superconductors magnetic properties; ferromagnetic and antiferromagnetic materials

Optical properties; photoconductivity, photovoltaic effect, applications, luminescence. Electrical properties: dielectric properties, piezo-electricity, Ferro electricity. Lasers and their applications in chemistry.

Preparative methods: Solid state reaction, chemical precursor method, co-Precipitation, sol-gel, metathesis, self-propagating high temperature synthesis, ion exchange reactions, intercalation/deintercalation reactions; hydrothermal and template synthesis.

References

1. F. A. Cotton, G. Wilkinson, C. A, Murillo, and M. Bochmann,Advanced Inorganic Chemistry, 6th Edn.,Wiley-Interscience: New York, 1999.

2. J.E. Huheey, E. A. Keiter and R. L.Keiter "Inorganic Chemistry, Principles of structure and Reactivity", 4thEdn.,Harper Collin College Publishers, 1993
3. G. Friedlander, J. W. Kennedy, E. S. Marcus andJ. M. Miller, Nuclear and Radiochemistry, John Cliffs, NJ, 1969.
4. L.V. Azaroff "Introduction to Solids" Mc.Graw Hill, New York,1960.
5. A.K. Galwey, Chemistry of Solids, Chapman and Hall, London, 1967.
6. L. Smart and E. Moore, Solid State Chemistry, Chapman and Hall, 1995.
7. H. V. Keer, Principles of the Solid State Wiley Eastern Ltd, New Delhi, 1993.
8. A. R. West, Solid State Chemistry and its Applications John Wiley & Sons, 1987.
9. A. K. Cheetham and P. Day (ed.), Solid State Chemistry-Techniques, Clarendon Press, Oxford, 1987.
10. D.K. Chakravarty, Solid State Chemistry, New Age International (p) Ltd.,Publishers, NewDelhi.1996.

Course Outcome:

- Develop a problem-solving approach in the main group, coordination and solid-state chemistry.
- To provide an introduction to the concepts underlying solid state chemistry.
- To illustrate the wide range of materials and their physical properties

CHE 5102 Organic Structure, Reactivity and Mechanism

Organic Structure, Stereochemistry and Reactivity

Molecular chirality, prostereoisomerism, stereotopicity and stereo projections. Non-carbon chiral centres. Atropisomerism and its designation. Stereoselectivity and asymmetric synthesis. Aromaticity. Aromatic annulenes, mesoionic compounds, azulenes, sydnones, fullerenes, metallocenes, cyclic aromatic carbocations and carbanions.

Reaction Mechanisms and Reactive Intermediates

Types of organic reactions and mechanisms. Reaction profiles and co-ordinates, kinetic and thermodynamic control. Hammond's postulate. Hammett equation and its application. Concerted and multistep reactions. Methods for the determination of reaction mechanisms. Intermediates in organic reactions. Structure, stability, formation and reactions of carbenes, nitrenes, carbon radicals, carbocations and carbanions.

Organic Reactions of sp3 Carbon Systems

Stereochemical and mechanistic aspects of SN reactions. Effect of solvent, leaving group and substrate structure. Neighbouring group participation. Nonclassical carbocations and ion pairs in SN reactions. Ambident nucleophiles and substrates. SN′ and SNi reactions. Elimination reactions leading to C=C bond formation. E1, E2 and E1cB mechanisms. Hoffman and Saytzeff modes of elimination. Effect of leaving group and substrate structure. Cis eliminations.

Organic Reactions of sp2 Carbon and Aromatic Systems

Electrophilic addition to C=C: Reactions and their mechanistic and stereochemical aspects. C=O based and C=O activated reactions. Named reactions based on C=O group. Stereochemistry of addition to C=O systems. Cram's rule. Felkin-Anh Model. Mechanism of esterification and ester hydrolysis. Aromatic electrophilic and nucleophilic substitutions. Electronic and steric effects of substituents. SN1, SNAr, Benzyne and SRN1 mechanism and their evidences. Radical additions, substitutions and chain reactions.

References

1. F. A. Carey, R. J. Sundberg (Part A and B), Kluwer Academic, 2000.
2. E. L. Eliel, Stereochemistry of Carbon Compounds, Wiley, 1997.
3. C. J. Moody, G. H. Whitham, Reactive intermediates, OUP primer, 1992.
4. R. Bruckner, Advanced Organic Chemistry – Reaction Mechanisms, Academic, 2003.
5. P. Sykes, A Guidebook to Mechanism in Organic Chemistry, 6th Ed., 1996.
6. T. H. Lowry, K. S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd Ed., Harper Row, 1997.

7. M. B. Smith, J. March, March's Advanced Organic Chemistry, 6th Ed., Wiley, 2012.
8. J. Clayden, N. Geeves, S. Warren, Organic Chemistry, OUP, 2001.

Course Outcome:

- Analyze the role of reactive intermediates such as carbocations and carbanions in chemical reactions.
- Classify, explain, and apply fundamental reactions. Be able to recognize, classify, explain, and apply fundamental organic reactions such as S_N2, S_N1, E2, E1, alkene addition, electrophilic aromatic substitution, 1,2/1,4-additions, ring-opening, and radical halogenation.
- Assess structural effects of organic molecules and functional groups on the tendency to participate in various types of organic reactions.

CHE 5103 Symmetry and Group Theory

Molecular Symmetry

Algebraic Systems. Common properties of operators. Levels of Abstraction.Subsystems. Direct Products. Isomorphisms. Axioms and theories of group. Abelian and cyclic groups. Finite sub-groups and Homomorphisms. Similarity Transformation and Classes. Cosets and Permutation Groups. Symmetry groups symmetry elements and operations. Planes, Axes, Inversions, Improper Axes. Products of symmetry operations. Equivalence symmetry elements and operations. Relations between symmetry operations. Classes. Symmetry groups with multiple higher order axes. Symmetry Point groups. Matrix representation of symmetry operations.

Applications of Group Theory in Chemistry

Representation of groups. Character. Reducible and irreducible representations. Great Orthogonality Theorem. Construction of character Tables.C3, C2v, C3v C4v, D3h, D4h Cyclic groups.

Applications of Group theory in bonding

C2v, C3v, D3h, D4h, Td. Conjugated systems and HMO method. Applications in spectroscopy IR, Raman and electronic spectra.

Symmetry in Crystallography

Point symmetry operations. Hexagonal Coordinates. Crystals systems. Lattice, primitive unit cell, Bravais lattices. Centering of lattices. Wigner-Seitz and other unit cells. 2d lattices. Crystallographic point groups. Schoenflies approach. Laues groups–space groups–symmorphic and non-symmorphic operations. Derivation of Space group.

References

1. F. A. Cotton, Chemical Applications of Group Theory, Wiley Eastern, 1985.
2. A. M. Lesk, Introduction to symmetry and group theory for chemists, Kluwer, 2004.
3. A. Vincent, Molecular Symmetry and Group theory, A Programmed Introduction to chemical applications, Wiley, 2001.
4. V. Ramakrishnan and M.S. Gopinathan, "Group Theory in Chemistry", Vishal Publications.
5. H. H. Jaffe and M. Orchin, "Symmetry in Chemistry", Wiley.

Course Outcome:

- Determine the symmetry elements of small and medium-sized molecules and apply point group theory to the study of electrical, optical and magnetic properties and selection rules for spectroscopy.

- Learn the basics of group theory and its application in chemistry.
- Understand the basic concepts of symmetry and its mathematical formulation.
- Apply these mathematical notations on objects and molecules.
- Analyze infrared, Raman, and electronic spectra of simple molecules.

CHE 5104 Quantum Chemistry

Introduction to Quantum Mechanics:

Particle aspect of radiation, black body radiation, photoelectric effect, Compton Effect, Molar Heat Capacities, Atomic and Molecular Spectra, Matter Waves and Heisenberg Uncertainty Relation etc.

Postulates:

Postulates of Quantum Mechanics, Operator Algebra, Schrödinger equation and nature of its solutions. Orthogonality and normalization. Stationary statesEnergies and degeneracies.

Model Systems:

Particle in 1D box, 3D box. Simple Harmonic Oscillator, particle in a ring. Angular momentum, rigid rotor.

Quantum Tunneling:

Particle encountering a barrier, tunneling. Tunneling in Chemistry, free particle

H atom:

Solution, quantum numbers and their interdependence. Radial and radial distribution plots, angular/polar plotsand spherical harmonics.

Approximation Methods:

Time independent perturbation theory. Non-degenerate states - First and second order perturbations. Application to particle in 1D-box, ring with $\cos 3\varphi$.

Variation theorem and its proof. Application to particle in 1D-box, stark effect, He atom by variation method.

Many Electron Wave Functions

Product wave functions. Nature of exchange. Electron spin, spin operators and spin Eigen Functions. Pauli's principle. Slater determinants.

Atomic Structure - Theory of Self-Consistent Field. HartreeFock Theory. SCF total electronic energy – Slater type orbitals. Aufbau principle, electronic configuration. Electron rules for atomic spectra. Periodic properties.

Hydrogen Molecule ion, Born Oppenheimer approximation, LCAO MO method.

Bonding in Diatomic Molecules

VB and MO methods of bonding. Bonding in polyatomic molecules. Spectroscopic term symbols of diatomic molecules, Non-crossing rule. Approximation methods in bonding in molecules. HMO method as applied to ethylene, allyl systems, butadiene and benzene.

References

1. D. A. McQuarrie, Quantum Chemistry, OUP, 1983.

2. J. P. Lowe, K. A. Peterson, Quantum Chemistry, Elsevier Academic, 2006.
3. P. W. Atkins, R. S. Friedman, Molecular Quantum Mechanics, OUP, 2005.
4. I. N. Levine, Quantum Chemistry, Prentice Hall, 2000.
5. A. K. Chandra, Introduction to Quantum Chemistry, Tata McGraw-Hill, 1988.
6. F. L. Pilar, Elementary Quantum Chemistry, 2nd Ed., McGraw-Hill, 1990.
7. J. Simons, An Introduction to Theoretical Chemistry, Cambridge University Press, 2003.
8. L. Pauling, E.B. Wilson, Introduction to Quantum Mechanics, McGraw-Hill, 1985.

Course Outcome:

- Use mathematical techniques in linear algebra for eigenvalues and eigenvectors and first and second order differential equations not only in quantum chemistry but in other areas of physical and theoretical chemistry that will be offered during the whole programme.
- Solve all the model problems in quantum mechanics for which exact analytical methods and solutions are available and apply them to analyze the basis behind the postulatory methods of quantum mechanics which form the foundations for advanced study of the subject.

CHE 5191 Inorganic Chemistry (Laboratory– I)

Reactions of titanium, vanadium, chromium, manganese, iron, cobalt, nickel and copper ions Reactions of some less common metal ions (Tl, W, Mo, V, Zr, Th, U). The spot test technique for metal ions. Semimicro qualitative analysis of common and rare cations in a mixture. Ion exchange separations (Zn^{2+}, Mg^{2+}). Solvent extraction (Fe). An open-ended experiment involving analysis (e.g., Double salt formation and ion-exchange separation of oxidation states). Estimation of metal ions by complexometric and cerimetric titrations. Estimation of Mg, Ca, Mn, hardness of water.

References

1. G. Pass and H. Sutcliffe. Practical Inorganic Chemistry, 2ndEdn., Chapman & Hill, 1974.

Course Outcome:

- Students will be trained to carry out the experiments on their own which helps them to attain more technical / practical skills.
- Apply essential chemical concepts and math skills toward successful completion of future science and applied science courses.
- They will understand how to estimate / quantify the presence of metal ions in a given mixture.

CHE 5192 Organic Chemistry (Laboratory-I)

1. Purification of liquids: Simple & fractional distillation methods
2. Purification of solids: Sublimation& recrystallization (benzoic acid, salicylic acid etc.)
3. Thin layer chromatography: Identification of known, unknown compounds and natural products and calculation of R_F and R_T values.
4. Paper Chromatography for separation of natural products – spinach, neem etc.
5. Polarimetry- Determination of the concentration of lactose, glucose, sugar etc.
6. Refractometry - Identification of pure organic liquids and oils. Determination of molar refractions of pure liquids. Determination of concentration of solutions.
7. Separation of a mixture of two components by solvent extraction.
8. Separation of organic compounds by column chromatography.
9. Determination of melting points of known and unknown compounds and the effect of impurities.
10. Single step organic synthesis – Nitration, bromination, amination etc.
11. Organic Synthesis- new reagents
12. Organic Synthesis - new methodology (macro, microscale etc.)
13. Characterization of organic compounds by UV and IR Spectroscopy.

References

1. A. I. Vogel, Practical Organic Chemistry, 5th Ed, 1989.
2. C. E. Bell, D. F. Taber, A. K. Clark, Organic Chemistry Laboratory, Thomson, 2000.
3. C. E. Bell, D. F. Taber, A. K. Clark, Organic Chemistry Laboratory with Qualitative Analysis, 3rd Ed., Brooks/Cole-Thomson Learning, 2001.
4. D. J. Pasto, C. R. Johnson, M. J. Miller, Experiments and Techniques in Organic Chemistry, Prentice Hall, 1991.
5. V. K. Ahluwalia, R. Aggarwal, Comprehensive Practical Organic Chemistry Vol. 1 & 2, Univ. Press, 2001.

Course Outcome:

- Learn how to separate and purify products in organic reactions.

- Students will demonstrate safe laboratory practices through the use of appropriate personal protective equipment and appropriate handling of all chemicals, including proper disposal of waste.
- Students will be trained to develop experimental and analytical skills to perform basic organic chemistry experiments.

Semester II

CHE 5201 Coordination Chemistry

Coordination Chemistry: Isomerism and nomenclature of coordination compounds. Stability of complex ions in solutions, stepwise formation of complexes, principles of determination of stability constants; chelate effect; concept of hard and soft acids and bases. Stabilisation of unusual oxidation states-stereochemistry of coordination compounds

Ligand field theory. Octahedral, tertrahedral and lower symmetry ligand fields. High spin and low spin complexes. Jahn-Teller effect. Application of group theory to construct correlation diagrams. Spectrochemical and nephelauxetic series. Molecular orbital theory. Ligand orbital combinations for octahedral and tetrahedral complexes. MO-correlation diagrams. Some illustrative examples: MnO_4^{-}, $Fe(CN)_6^{2-}$, $Fe(bpy)_3^{2-}$, $Ru(bpy)_3^{2-}$, $Ni(CO)_4$, $Fe(C_5H_5)_2$.

Magnetism, orbital contribution, spin orbit coupling and covalency. Dia, para, ferro and antiferro magnetism, quenching of orbital angular momentum. Spin crossover systems. Magnetic properties of lanthanide ions. Electronic spectra of transition metal complexes. Orgel and Tanabe-Sugano diagrams. Charge transfer transitions.

Substitution reactions. Inert and labile compounds, dissociative, associative, aquation, and conjugate base mechanism. Trans effect, trans effect series, and theories of trans effect. Electron transfer reactions. Inner sphere and outer sphere mechanisms.

References

1. D. F. Shriver, P. W. Atkins and C. H. Langford, Inorganic Chemistry, 3rd Edn., ELBS, 1999.
2. F. A. Cotton andG. Wilkinson, Advanced Inorganic Chemistry, 5thEdn., Wiley.
3. J. E. Huheey, Inorganic Chemistry, 4thEdn., Harper Intl.
4. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rdEdn., Wiley.
5. N. N. Greenwoodand A. Earnshaw, Chemistry of the Elements, 2nd Edn., BH, 1997.
6. W. L. Jolly, Modern Inorganic Chemistry, 2nd Edn., McGraw-Hill, 1991.

Course Outcome:

- An overview of the theories of bonding in coordination complexes.

- Describe CFSE, high and low spin complexes, magnetic moment of coordination compounds etc.
- Recognition of the types of isomers in coordination compounds.
- Knowledge of the reactions and electronic spectral properties of coordination complexes.

CHE 5202 Organic Reactions and Synthesis

Symmetry Controlled Reactions and Organic Rearrangements

Theory, mechanism and stereocourse of electrocyclic, cycloaddition and sigmatropic reactions. Woodward-Hoffmann selection rules. Cheletropic and ene reactions. 1,3-dipolar cycloadditions. Anionotropic, cationotropic, prototropic, free radical, carbene, nitrene and long-range rearrangements. Migratory aptitudes. Rearrangements involving C→C, C→N, C→O and hetero atom→C migrations. Migration of H, alkyl, aryl, hetero atom and other groups.

Organic Photochemistry

Primary photoprocesses. Photoreactions of C=O systems, enes, eneones (acyclic and cyclic), dienes and arenes. Photoisomerisations and rearrangements. Norrish type I and II, photo-Fries, Patterno-Buchi and Barton reactions. Di-pi methane and aromatic photo rearrangements. Photochemical remote functionalisation. Introduction to PET, chemi, bioluminescent and singlet oxygen reactions. Photosynthesis. Hoffman-Loeffler-Freytag reaction. Photochemistry of Vit D and Vit A.

Organic Synthesis

Introduction to retrosynthetic analysis. Linear and convergent synthesis, Synthons, functional group equivalents and umpolung. Chemo, regio and stereoselectivity in reactions. Classical and modern carbon-carbon (C-C and C=C) and carbon-hetero atom bond forming reactions in organic synthesis. Enolates and enamines and their alkylations in C-C bond formations. Control of enolate formation. Kinetc and thermodynamic enolates. Functional group interconversions. Baylis-Hilman, Sonogashira reaction. Glaser coupling, Shapiro, Peterson, Heck, Stille, McMurray, Wittig and related reactions. Organometallic (Li, Mg, Hg, Zn, Cu) and organo-nonmetallic (B, P, Si) reagents in organic synthesis. Ylides and their applications. Hydroboration and transformation of alkylboranes.

Reduction and Oxidation in Organic Synthesis

Catalytic hydrogenation and stereochemistry. Hydrogenation catalysts and their selectivity. Homogeneous hydrogenations. Fe, Zn, Na and Li reductions. Hydrides reductants. LAH, $NaBH_4$ and $NACNBH_3$. Dehydrogenation to aromatic compounds. Oppenauer oxidation. Oxidations using SeO_2, lead tetraacetate, ozone, HIO_4, OsO_4 and peracids. Sommelet reaction. Dehydrogenation to aromatic compounds. Swern oxidation, Moffatt oxidation, allylic and benzylic oxidations. Sharpless assymetric epoxidation. Elbs reaction. Oxidative coupling of phenols. Epoxidation of C=C using peracids. Conversion of epoxide to alkenes. Prevost and Woodward procedures for diols. 1,2-Diols and their oxidative cleavage.

References

1. R. K. Mackie, D. M. Smith and R. A. Aitken, Guidebook to Organic Synthesis, Longman 3rd Edn.
2. V. K. Ahluwalia and R. Aggarwal, Organic Synthesis: Special Techniques, Narosa.
3. R. O. C. Norman and A. Coxon, Modern Synthetic Reactions, Chapman and Hall
4. P. R. Jenkins, Organometallic Reagents in Synthesis, OU Primer 3, OUP.

Course Outcome:

- Understand different types and distinctive features of advanced organic reactions and reagents.
- Understand the advanced concepts related to the structure and properties of various organic reagents and compounds.
- Apply resonance and conjugation concepts. Predict and explain patterns in stability, shape, hybridization, reactivity, and product formation when resonance or conjugation applies to a reactant, intermediate, or final product.

CHE 5203 Thermodynamics, Kinetic Theory and Statistical Mechanics

Thermodynamics

Laws of thermodynamics. Need for second and third laws. Entropy and free energy functions Nernst heat theorem. Apparent exceptions to and applications of third law. Thermodynamics of irreversible processes. General theory of nonequilibrium processes. Entropy production. Flux-force relationship. Onsager reciprocal relations. Application to the theory of diffusion, thermal diffusion, thermoosmosis and thermomolecular pressure difference. Electrokinetic effects. The Glansdorf-Pregogine equation.

Kinetic Theory

Brownian movement. Determination of Avogadro number. Distribution of molecular velocities. Maxwell's equation. Average and most probable velocities from Maxwell equation. Influence of temperature. Mean free path. Collision diameter. Triple collision. Viscosity. Thermal conductivity and diffusion. Determination of viscosity of gases. Influence of temperature and pressure on transport properties.

Statistical Thermodynamics

Mechanical description of molecular systems. Microstates. Canonical and grand canonical ensembles. Equation of state for ideal quantum gases. Maxwell Boltzman distribution. Partition functions. Partition functions and thermodynamic properties. Heat capacity of gases. Equipartition principle and quantum theory of heat capacity.

Quantum statistics

Bose Einstein statistics. Theory of paramagnetism. Bose-Einstein condensation. Fermi Dirac statistics. Thermionic emission. Relations between Maxwell-Boltzman, Bose-Einstein and Fermi-Dirac statistics. Heat capacity of solids. The vibrational properties of solids. Einstein theory of heat capacity. The spectrum of normal modes. The Debye theory. The electronic specific heat.

References

1. Clotz and Rosenberg Chemical Thermodynamics Academic Press.
2. J. Rajaram and J. C. Kuriacose, Thermodynamics, S N C & Co.
3.J. W. Sears and Salinger, Introduction to Thermodynamics, Kinetic Theory & Statistical Themodynamics, Addison Wesley Pub.
4. A Course in Statistical Thermodynamics, J Kestin & J R Dorfman, Academic Press.
5. L. K. Nash, Statistical Thermodynamics, Addison Wesley.
6. Introduction to Irreversible Thermodynamics, Prigogine, Interscience.

Course Outcome:

- Understanding the fundamentals of chemical thermodynamics.
- Solving problems related to the feasibility of a physical/chemical processes.
- Correlation of thermodynamics with quantum mechanics.

CHE 5204 Molecular Spectroscopy

Electromagnetic radiation, interaction of electromagnetic radiation with matter, quantum mechanical approach - transition probabilities: Einstein coefficients

Microwave and IR Spectroscopy:

Pure vibrational and rotational spectra, selection rules, vibrational and rotational spectra of polyatomic molecules, normal modes, anharmonicity, selection rules - Raman effect: classical and quantum theory of Raman effect, rotational and vib-rotational Raman spectra.

Electronic Spectroscopy:

Spectroscopic term symbols, transition moments, assignment of electronic transitions of N2, H2O and formaldehyde using group theory, fluorescence and phosphorescence, ESCA, PES, AUGER techniques.

Introduction to NMR:

Origin of magnetic moments in matter, electronic and nuclear moments, interaction with magnetic field, Larmor equation - conditions for magnetic resonance absorption, FT techniques, T1 and T2 relaxation times, line widths and line shapes, chemical shifts, ring currents, diamagnetic anisotropy, spin-spin splitting, high resolution NMR spectra of simple molecules, first and second order treatment of AB systems.

Other Resonance Spectroscopy Methods:

Electron Spin Resonance: g- value, hyperfine structure, ESR of organic free radicals, solids, inorganic ions, and simple free radicals. NQR and Mossbauer spectroscopic techniques.

References

1.A. Carrington, A. D. McLachlan, Introduction to Magnetic Resonance, Harper & Row, New York, 1979.

2. A. Derome, Modern NMR Technique, Pergamon, 1983.
3. J. E. Wertz, J.R. Bolton, Electron Spin Resonance, McGraw-Hill, 1972.
4. P. W. Atkins, Physical Chemistry, 10th Ed., Oxford, London, 2014.
5. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, 2nd Ed., Saunders, 1996.
6. C. N. Banwell, Molecular Spectroscopy, Tata McGraw-Hill, 1998.
7. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw-Hill, 1964.
8. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw-Hill, 1998.

Course Outcome:

- Prediction of the allowed transitions between various molecular energy levels.

- Understand the theoretical basis of rotational, vibrational and Raman spectroscopy.
- Application of vibrational and rotational spectroscopy for the structural elucidation of chemical compounds.
- Principles of ESCA, PES, AUGER, NMR, EPR, Mossbauer spectroscopy and NQR.

CHE 5291 Physical Chemistry (Laboratory– I)

This laboratory course covers basic physical chemistry experiments employing minor or major equipment and computational facility that are available in the Department/sister Department.*

General Experiments: Phase diagram of a three-component system, Adsorption of acetic acid on charcoal, Kinetics of iodine clock reaction, Study of persulphate-iodide second order reaction, Determination of first order rate constant - acid hydrolysis of an ester, Critical solution temperature (CST), Conductometric titrations of mixture of acids, Conductometric titration of a charge transfer complex, Estimation of CMC of a micelle from conductance measurements, Potentiometric titration of a redox reaction, Estimation of ferrous ions by potentiometry, Validation of Beer Lamberts law by FTIR spectrometer, Validation of Beer Lamberts law by UV-visible spectrometer.

Computational Chemistry Experiments: Study of normal modes, Determination of equilibrium constants, Determination of rate constants.

Supplementary experiments: Conductometric titrations of acid & base, Determination of second order rate constant – Base hydrolysis of ester, Study of an oscillating reaction, Determination of isoelectric point of amino acid by pH metric titration, Estimation of mixture of acids by pH metric titration by using NaOH, Estimation of phosphoric acid by pH metric titration, Equilibrium constants of tri-iodide and copper-ammonium complexes, Enthalpy change for tri-iodide formation, Determination of unknown sugar solution concentration by polarimeter, Determination of Activation energy and Arrhenius parameters, Open-ended lab experiment.

*Minimum of twelve experiments can be selected from general and computational chemistry experiments. Additional experiments can be selected from general or supplementary experiments or any other of course instructor's choice that falls under the title of the course for which procedure is well known in the literature:

References

1. *Laboratory Manual*, 2013, Department of Chemistry, Central University of Kerala.
2. A. J. Elias, *General Chemistry Experiments*, University Press, Hyderabad, 2002.
3. F. Daniels, J. W. Williams, P. Bender, R. A. Alberty, C. D. Cornwell, J. E. Harriman, *Experimental Physical Chemistry*, McGraw-Hill, 1962.
4. R. C. Das, B. Behera, *Experimental Physical Chemistry*, Tata McGraw-Hill, 1993.
5. D. P. Shoemaker, C. Garland, J. W. Nibler, *Experiments in Physical Chemistry*, McGraw-Hill, New York, 1996.
6. D. C. Young, *Computational Chemistry*, John-Wiley and Sons, NY, 2001.
7. MOPAC 6.0 *Manual and Computer program*, QCPE Ed., 2012.

8. PCMODEL *Manual and Computer program*, Serena Software, 2011

Course Outcome:

- Understand the fundamental theories of experimental physical chemistry.
- Recognize the role of multidisciplinary streams starting with basic science to understand the key role of instruments in doing experimental physical chemistry.
- Develop problem-solving and troubleshooting ability in experimental physical chemistry, and to nurture experimental and analytical skills suitable for research in the area of physical chemistry.

CHE 5292 Organic Chemistry (Laboratory-II)

One step or multistep organic synthesis, estimation and characterization of the synthesized compounds by various analytical methods.

1. Preparative chromatographic separation of organic compounds
2. Elemental analysis of organic compounds
3. Isolation of natural products- Plant extracts
4. Extraction of oils- Peanut oil, Castor oil, Neem oil etc.
5. Estimation of amino acids by chemical methods
6. Estimation of nitrogen by Kjeldahl method
7. Radical reactions – Free radical addition (polystyrene, polymethylmethacrylate, PVA etc.)
8. Oxidation of primary and secondary alcohols
9. Cycloaddition – Diels Alder Reactions
10. Synthesis of pharmacologically active compounds – Aspirin, Acetaminophen etc.
11. Esterification of alcohols (example: n-butyl alcohol)
12. Rearrangement reaction – Beckman rearrangement of acetopheonone oxime
13. Electrophilic, nucleophilic reactions
14. Photochemical Reactions
15. Enzymatic reactions
16. Multistep synthetic reactions
17. Quantitative determination of organic compounds, amino acids, and proteins using spectrophotometric methods.
18. GC Analysis of organic compounds
19. HPLC Analysis of organic compounds and biomolecules

References:

1. A. I. Vogel, Practical Organic Chemistry, 5th Ed, 1989.
2. C. E. Bell, D. F. Taber, A. K. Clark, Organic Chemistry Laboratory, Thomson, 2000.
3. C. E. Bell, D. F. Taber, A. K. Clark, Organic Chemistry Laboratory with Qualitative Analysis, 3rd Ed., Brooks/Cole-Thomson Learning, 2001.
4. D. J. Pasto, C. R. Johnson, M. J. Miller, Experiments and Techniques in Organic Chemistry, Prentice Hall, 1991.
5. V. K. Ahluwalia, R. Aggarwal, Comprehensive Practical Organic Chemistry Vol. 1 & 2, Univ. Press, 2001.

Course Outcome:

- Separation and purification of organic compounds by employing chromatographic techniques.
- Separate/purify organic liquids/solids by using standard methods.

- Acquire skills to perform organic synthesis, separation and purification of products, followed by characterization using instrumental spectroscopic methods, which will be helpful to pursue research career in organic chemistry/organic synthesis.

Semester III

CHE 5301 Organo-metallic and Bio-inorganic Chemistry

Compounds with transition metal to carbon bonds: classification of ligands, nomenclature, eighteen electron rule; transition metal carbonyls: structure, bonding, spectra, preparation and reactions; transition metal organometallics. Metal-olefin and arene metal bonds. Transition metal clusters. Isoelectronic and isolobal relationships. Metal nitrosyls,cyanides: and isocyanides.

Organometallic reactions and catalysis: oxidative addition, reductive elimination, insertion, hydride elimination, abstraction; olefin hydrogenation, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, olefin isomerisation, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation.

Metal ions in biological systems: heme proteins, hemoglobin, myoglobin, hemerythrin, hemocyanin, ferritin, transferrin, cytochromes and vitamin B12; Iron-sulphur proteins: rubredoxin, ferredoxin and model systems.

Metalloenzymes: active sites, carboxy peptidase, carbonic anhydrase, superoxide dimutase, xanthine oxidase, peroxidase and catalase; photosynthesis, water oxidation, nitrogen fixation, nitrogenase; ion pump, metallodrugs.

References

1. P. Powell, Principles of Organometallic Chemistry, 2^{nd}Edn., ELBS, 1991.
2. J. E. Huheey, Inorganic Chemistry, 4th Edn., Harper International, 2001.
3. R. G. Wilkins, Kinetics and Mechanism of Reactions of Transition Metal Complexes, 2Edn, VCH.
4. R. W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987.
5. R. H. Crabtree, The Organometallic Chemistry of Transition Metals, 2^{nd}Edn., Wiley.
6. A. W. Parkins and R. C. Poller, An Introduction to Organometallic Chemistry, Macmillan
7. J. A. Cowan, Inorganic Biochemistry - An Introduction, VCH.
8. I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, Bioinorganic Chemistry, Viva Books.

Course Outcome:

- Understand the structure, bonding, reactivity including safe handling of various organometallic compounds.
- Understand and apply the various organometallic compounds for catalytic applications relevant to chemical and polymer industries.
- Explain the function of various elements in biological systems.

CHE 5302 Organic Spectroscopy and Bio-organic Chemistry

Heterocyclic and Bioorganic Chemistry

Aromatic heterocyclic compounds – five and six membered heterocyclic systems with two Hetero atoms (N, O, S). Benzo fused heterocyclic systems – structure, synthesis and reactivity. Amino acids: codes. Peptide bond formation methods, amino and carboxy protection. Solid Phase Peptide Synthesis. Purines and Nucleic acid bases. Synthesis of adenosine, ADP and ATP. Primary, secondary and tertiary structure of proteins and DNA. Vitamins and their chemistry – Vit A, Vit B1, B2, Vit C and Vit E.

Natural Products Chemistry

Classes, typical examples and structures of secondary metabolites. Chemical and spectroscopic methods for establishing carbon skeleton, functional groups and stereochemistry of natural products. Structure of typical terpenoids such as pinene, camphor, abietic acid and squalene. Structure of steroids cholesterol, stigmasterol, estrone, progesterone, testosterone. Chemistryof polyphenolics. Structure determination of representative examples of pyrrolidine, piperidine, indole, quinoline, and isoquinoline alkaloids; Structure of beta-lactam antibiotics–penicillin G.

Organic NMR spectroscopy

^{1}H and ^{13}C NMR chemical shifts and coupling constants. Proton coupled; off–resonance decoupled; proton noise decoupled ^{13}C NMR spectra. Coupled spin systems. Structure information derived from δ and J values. Spin systems and their analysis. Tree diagram. Chemical exchange, double resonance, NOE and DEPT. Introduction to 2D NMR. Correlation, NOE and quantum correlation spectroscopy techniques.

Organic structure by spectroscopy

UV-VIS spectra of enes, eneones, arenes and conjugated systems. Solvent effect on absorption spectra.Solvatochromism. Application of ORD and CD. Identification of functional groups and other structural features by IR. MS in organic structure analysis. Basic principles, mass analyzers, ionization methods: EI, PI, CI, FAB, MALDI, ES. Characteristic EIMS fragmentation modes and MS rearrangements. Spectral interpretation, structure identification and solving of structural problems using numerical and spectral data.

References

1. J. A Joule and K.Mills, Heterocyclic Chemistry, 4thEdn., Blackwell, 2000.
2. J. R. Hanson, Natural products: Secondary Metabolites, RSC.
3. J. Mann and others, Natural Products: Chemistry and Biological Significance, Longman.
4. J. Mann, Chemical Aspects of Biosynthesis, Oxford primer 20, OUP.

5. R. J. Simmonds, Chemistry of Biomolecules, RSC.
6. S. V. Bhat, B. A. Nagasampagi and M. Sivakumar, Chemistry of Natural products, Narosa, 2005.
7. R.H. Thomson, Chemistry of Natural Products - Wiley, New York, 1996.
8. I. L. Finar, Advanced Organic Chemistry, ELBS, New Delhi, 1975.
9. D. Voet and G. J. Voet, Biochemistry, Wiley.
10. D. L. Pavia, G. M. Lampman and G. S. Kriz, Introduction to Spectroscopy.
11. D. H. Williams and I. Fleming, Spectroscopic methods in organic chemistry,
12. R. M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds, 6th Edn., Wiley.
13. W. Kemp, Organic Spectroscopy, 3rd Edn., MacMillon, 1994.
14. V. K. Ahluwalia, L. S. Kumar and S. Kumar, Chemistry of Natural Products Ane Books.

Course Outcome:

- Describe the basic principles and applications of organic-mass spectrometry.
- Describe the applications of UV-Visible spectroscopy in the identification of π-conjugation in organic compounds
- Evaluate the structure of organic compounds using ^{1}H, ^{13}C, and 2D-NMR spectroscopy.

CHE 5303 Reaction dynamics, surface and electro chemistry

Chemical Kinetics and Catalysis

Order and molecularity of reactions. Complex reactions. Reversible, consecutive, concurrent and branching reactions. Free radical and chain reactions. Steady state treatment. Rice-Herzfeld mechanism. Unimolecularreaction. Lindemann treatment. Semenoff-Hinshelword mechanism of chain reactions and explosion. Fast reaction kinetics. Methods to study kinetics of fast reactions. Catalysis: Mechanism and theories of homogeneous and heterogeneous catalysis. Acid-base and enzyme catalysis. Langmuir Hinshelwood mechanism.

Reactions in solutions

Factors governing rates of reaction in solution. Theories of reactions in solutions. Solvent polarity. Solvent polarity scales. Kinetic isotope and solvent isotope effects. Hammett and Taft equations. Linear free energy relationships. Primary and secondary effects. Salt effects and special salt effects. Phase transfer Catalysis.

Reaction Dynamics

Potential energy surfaces. Electronically excited molecules, bimolecular collisions, molecular beam scattering, statistical approach of reaction dynamics to transition state theory, unimolecular reaction dynamics, transition state theory of solution reactions, Kramers's theory.

Surface Chemistry

Types of surfaces. Thermodynamics of surfaces. Measurements of surface pressure and surface potential. Surfactants and micelles. The gas-solid interface. Types of adsorption. Gibbs adsorption equation. Langmuir isotherm. Multilayer adsorption. Freundlich isotherm. BET isotherm. Measurements of surface area of solids.

Electrochemistry

Ionic activity. Ion transport. Debye-Huckel treatment. Onsager equation. Electrodes and electrochemical cells. Liquid junction potential. Evaluation of thermodynamics properties. Electrokinetic phenomena. Over potential. Butler-Volmer, Tafel and Nernst equations. Electrical double layer, electrochemical reactions. Corrosion and its control. Introduction to solid state electrochemistry.

References

1. P. W. Atkins, Physical Chemistry, 8th Edn., OUP, 2006.
2. McQuirre, Physical Chemistry, 2ndEdn., Viva Publications, New Delhi, 2001.
3. Thomas, Engel and Reid, Physical Chemistry, Pearson Education India, 2006.

4. N. S. Issacs, "Physical Organic Chemistry", Longman.
5. A. W. Adamson, The Physics' and Chemistry of Surfaces, Interscience.
6. N. K. Adam, The Physics and Chemistry of Surfaces, OUP.
6. S. J. Gregg, The Surface Chemistry of Solids, Chapman Hall.
7. F. W. Sears, Introduction to Thermodynamics, Kinetic Theory of Gases and Statistical mechanics, Addison Wesley.
8. P. W. Atkins, Physical Chemistry, OUP.
9. D. R. Crow, The Principle of Electrochemistry, Chapman Hall.

Course Outcome:

- Overview of reaction kinetics, surface chemistry and electro-chemistry in terms of established theories.
- Development of problem-solving ability in electrochemistry, kinetics, and surface chemistry.
- Prediction of possible mechanisms involved in it.
- Theoretical understanding of how chemical reactions take place.

CHE 5391 Inorganic Chemistry (Laboratory– II)

Synthesis of inorganic complexes and their characterization by various physicochemical methods, such as IR, UV, Visible, NMR, magnetic susceptibility etc.

H_2 Salen-based complexes

Nickel (II) complexes of H_2 Salen

Copper (II) complexes of H_2 Salen

Cobalt (II) complexes of H_2 salen and its oxygen binding

Amine based Complexes

Hexamminecoblat(III) chloride

Pentamminechlorocobalt(III) chloride

Nitritopentamminecobalt(III) chloride

Nitropentamminecobalt(III) chloride

8-Hydroxyquinoline (L) based complexes

Aluminium (III) oxine $[Al^{3+}(L)_3]$

Iron (III) oxine $[Fe^{3+}(L)_3]$

Zinc (II) oxine $[Zn^{2+}(L)_3]$

Acetylacetonate based complexes

Vanadium (IV)oxy acetylacetonate

Tris(acetylacetonato) Manganese (II) / Tris(acetylacetonato) Manganese (III)

Tris(acetylacetonato) aluminium (III)

Tris(acetylacetonato) iron(III)

Tris(acetylacetonato) chromium (III)

Other complexes / materials

Potassium copper(II) oxalate complexes

Optical isomers of tris(ethylenediamine)cobalt(III)chloride

Tris(oxalate) manganese(III)

Tris(thiourea) copper(I) sulphate

Preparation of MnO_2 nanoparticles using Cetyltrimethylammonium bromide surfactant

Preparation of zeolite, clay materials

Preparation of potassium bis(peroxo)-oxo-(1,10-phenothroline) vanadium (V) trihydrate

Preparation of 12-tungstosilicic acid

Selection can be made from the above specified or any other complexes for which references are available in the literature.

Attempts will also made to interpretation of electronic spectrum of transition metal complexes and the calculation of Dq values. Determination of crystal field splitting energy for certain ligands and construction of a part of the spectrochemical series

References

1. G. Pass and H. Sutcliffe. Practical Inorganic Chemistry 2ndEdn.,Chapman& Hill. 1974.
2. G. Marr and B. W. Rockett. Practical Inorganic Chemistry, Van Nostrand, 1972.

Course Outcome:

- Understanding the strategies for the synthesis of various types of inorganic compounds.
- Synthesis and characterization of a new inorganic complexes.
- Develop laboratory and analytical skills required for carrying out synthesis in inorganic chemistry research.

CHE 5392 Physical Chemistry (Laboratory– II)

This laboratory course covers advanced physical chemistry experiments employing minor or major equipment and computational facility that are available in the Department/sister Department.*

General Experiments: Spectrophotometric determination of *p*Ka, Jobs plot and stoichiometry of a complex by mole ratio method, Kinetics of an enzyme-catalyzed reaction by spectrophotometer Bimolecular, Determination of excited state acidity constant, Rate constant by Stern-Volmer graph using fluorimeter, $CuSO_4$ and Calcium oxalate TGA study, Differential scanning calorimetric study (DSC), Determination of the unit cell of a crystal, Rate constant of mutarotation of glucose and fructose by polarimetry, Determination of concentration of Na and K by AAS, Qualitative and quantitative study by Gas chromatography, Redox potentials by Cyclic voltammetry.

Computational Chemistry experiments: Franck-Condon spectral calculations, Construction of Walsh diagram, Woodward - Hoffman correlation diagrams.

Supplementary Experiments: Photometric titrations, Additive principle by spectrophotometry, Estimation of CMC of a micelle using fluorescence, Determination of dipole moment change on electronic excitation, Identifying the nature of materials based on sorption isotherms, Open-ended lab experiment.

*Minimum of twelve experiments can be selected from general and computational chemistry experiments. Additional experiments can be selected from general or supplementary experiments or any other of course instructor’s choice that falls under the title of the course for which procedure is well known in the literature:

References

1. *Laboratory Manual*, 2013, Department of Chemistry, Central University of Kerala.
2. A. J. Elias, *General Chemistry Experiments*, University Press, Hyderabad, 2002.
3. F. Daniels, J. W. Williams, P. Bender, R. A. Alberty, C. D. Cornwell, J. E. Harriman, *Experimental Physical Chemistry*, McGraw-Hill, 1962.
4. R. C. Das, B. Behera, *Experimental Physical Chemistry*, Tata McGraw-Hill, 1993.
5. D. P. Shoemaker, C. Garland, J. W. Nibler, *Experiments in Physical Chemistry,* McGraw-Hill, New York, 1996.
6. D. C. Young, *Computational Chemistry*, John-Wiley and Sons, NY, 2001.
7. MOPAC 6.0 *Manual and Computer program*, QCPE Ed., 2012.
8. PCMODEL *Manual and Computer program,* Serena Software, 2011

Course Outcome:

- Apply the fundamental knowledge in experimental physical chemistry to existing and emerging problem in basic science.
- Recognize the role of multidisciplinary streams starting with basic science to understand the key role of instruments in doing experimental physical chemistry.
- Develop laboratory and analytical skills required for carrying out research work.

SEMESTER IV

CHE 5490 Dissertation / Project work

Students will be provided with short term research project of 3 months duration in the research laboratories of the department. They will have to design, execute, prepare documented report and present their work before an expert committee.

Course Outcome:

- Understand and identify new research problems in chemistry.
- Collect literature in the identified research area using scientific resources.
- Design the new synthetic scheme or protocol based on the literature search.
- Execute experiments/computations/theory to collect and analyze the data.
- Prepare the research report based on the obtained results, present and defend their work before an expert committee.
- Intended for acquiring skills in laboratory/computational experiments, in order to equip them to pursue research career.

ELECTIVE COURSES

(To be taken during the IIIrd & IVth Semester)

CHE 5001 Instrumental Methods of Analysis

Elementary electronics - semiconductors - properties - semiconductor diodes- transistors- mechanism of amplification- field effect transistors – transformers- rectifiers- voltage regulators – noise – signal - to – noise ratio - readout devices - cathode ray tube

Electrogravimetry - coulometry - constant current and constant potential coulometry- applications-primary and secondary coulometry – conductance measurement – conductometric titrations. Ion-selective electrodes, ion-selective FET, immobilized enzyme electrodes construction.

Polarography – current – voltage curve. DME-components of polarographic current – supporting electrolyte – polarographic maxima. Half-wave potential-Instrumentation- Applications of Polarography. Pulse and differential pulse polarography-chronopotentiometry - stripping analysis. Amperometric titrations – Different types. Applications. Cyclic voltrametry - Theory and applications.

UV-VIS and IR Spectrophotometry. Basic instrumentation for UV-Vis and IR spectrophotometry - single beam and double beam instruments, FT-IR, Fundamental laws of photometry - deviations from Beers law - photometric accuracy –relative photometric error– simultaneous determination of two components-. Nephelometry and turbidimetry.

Instrumentations of FT-NMR, advanced Mass Spectrometry including hyphenated techniques, introduction to X-ray diffraction.

Flame Emission and Atomic Absorption Spectrometer. Instrumentation of AAS, the flame spectra, flame characteristics. Atomizers used in spectroscopy, Hollow cathode lamp interference in AAS-applications. Atomic emission spectroscopy-flame photometry- simultaneous multi element analysis.

Chromatography-classification - column-paper and thin layer chromatography. HPLC -outline study of instrument modules. Ion – exchange chromatography - Theory. Important applications of chromatographic techniques. Gel Permeation Chromatography.

Gas chromatography–basic instrumental set up-carriers, columns, detectors and comparative study of TCD, FID, ECD and NPD. Qualitative and quantitative studies using GC, Preparation of GC columns, selection of stationary phases of GLC, Gas adsorption chromatography, applications, CHN analysis by GC.

Thermal methods of Analysis TG, DTA and DSC - Instrumentation and Theory – effect of atmosphere on TG and DTA. TG of copper sulphate pentahydrate and calcium oxalate monohydrate. Application of thermal methods for identification of substances.

Automated methods of analysis-advantages and disadvantages-types of automatic analytical systems- flow injection analysis- instrumentations – applications-discrete automatic systems.

References

1. D.A. Skoog and D.M West, Principles of Instrumental Analysis, 2nd Edn., Saunders college, Philadelphia, 1980.
2. Pecksock, Shields, Carrns and Mc William, Modern Methods of Chemical Analysis, John Wiley, 2nd Edn., 1976.
3. H.H. Willard , L.L. Merrit, J.A. Dean and F.A. Settle, Instrumental Methods of Analysis, D, Van Nonstrand, N.Y, 1981.
4. F.W. Fifield and D. Kealey, Principles and Practice of Analytical Chemistry, 2nd Edn., International Book Company, London, 1983.
5. Leitinon and W. Harris, Chemical Analysis, 2nd Edn., McGraw Hills, Tokyo, 1975.
6. H.A. Donald and F. Calbreath, Clinical chemistry- A fundamental text book, An HBJ international Edn., W.B. Saunders, 1992.
7. K. Wilson and J. Walker, Practical Biochemistry-Principles and Techniques, Cambridge University Press, 1995.

Course Outcome:

- Understanding of the fundamental principles of instrumental measurements.
- Application of these principles to specific types of chemical measurements (type of sample analysed, figures of merit, strengths and limitations).
- Use of instruments to solve real analytical problems.

CHE 5002 Chemistry of Biopolymers and Biochemical Reactions

Chemistry of automated polypeptide and oligonucleotide syntheses. Chemistry of protein and polynucleotide sequencing. Automated gene sequencing. Genome sequencing–a brief introduction.

Structure of polypeptides and proteins. Helical, sheet and random coil structures. Higher order structure and protein folding. Structure of collagen and introduction to Ramachandran plots.

Structure of polynucleotides. A-, B- and Z-DNA duplex structures. Base pairing and codon-anticodon recognition. Types of RNAs. Structure and folding in RNAs. Genetic code. Wobble hypothesis. Gene expression and protein biosynthesis. Recombinant DNA methods.

Chemistry of starch, cellulose, dextran and glycogen. Chemistry of sialic acid and introduction to glycochemistry. Basis of cell-cell recognition and blood group chemistry. Structure of Chitin.

Lipids and biomembranes. Classes of lipids with typical examples and their function. Lipid aggregates: micelle, bilayer, liposome and biomembrane formation. Structure of cell membranes and models. .

Introduction to Enzymes. Active sites and allosteric sites. Classification of enzymes. Mechanism of enzyme action. Trypsin, chymotrypsin, lipases and carboxypeptidases. Immobilized enzymes and enzyme technology.

ATP and biological energetics. Structure and function of NADH, NADPH, $FADH_2$,. Fixation of carbon dioxide and other photosynthetic reactions. Glycolysis. Kerb's cycle. Structure and reactions of important coenzymes. Kelvin cycle. Urea cycle. Biosynthesis of secondary metabolites – terpenes, alkaloids and steroids. Biosynthesis of amino acids.

Introduction to medicinal chemistry. Mechanism of drug action. Receptor and ligand interactions. Drug discovery and development methods. SAR. ADME. Typical examples of analgesics, anti-inflammatory agents, antipyretics, antihypertensives and antibiotics – structure and synthesis of simole examples.

References

1. R. J. Simmonds, Chemistry of Biomolecules, RSC.
2. H. Dugas, Bioorganic Chemistry, Springer.

CHE5003 Computational Chemistry

Molecular Mechanics. Potential energy surfaces. Curve crossing Model. Force field. Factors governing barrier heights. Quantum Mechanical and Molecular Mechanics potential functions. MM force fields. Parametrization. Steric energies, Heats of formation and strain. Compu-chem lab: Z-matrix specification, Input for Semi-empirical and *ab-initio* programs. Molecular mechanics program. Analysis of output.

References

1. F. Jensen, Introduction to computational chemistry, Wiley, NY, 2007.
2. D. C. Young, Computational Chemistry, John-Wiley and Sons, NY, 2001.
3. C. J. Cramer, Essentials of Computational Chemistry, John-Wiley & Sons, 2004.
4. U. Burkert and N.L. Allinger: Molecular Mechanics, ACS Monograph, American Chemical Society, 1977.
5. Albright, Burdett and Whanghbo, Approximate Molecular Orbital Theory, Academic Press, 1985.
6. MOPAC 6.0 Manual and computer program, QCPE Ed.
7. PCMODEL Manual and Computer program, Serena Software.

Course Outcome:

- Understanding of the basic principles of computational chemistry.
- Performance of simple computational experiments in energy evaluation, transition state modeling, conformational analysis.
- Skill development to design, perform and analyze chemistry problems using computational tools.

CHE 5004 Electro-analytical Techniques

Mass transfer by diffusion and migration, general mass transfer equations, Ionic migration and diffusion. Ilkovic equation, polarography, chronoamperometry, chronocoulometry, pulse polarographic methods.

Cyclic voltammetry: Nernstian reversible, totally irreversible, quasi-reversible processes, controlled potential methods, electrogravimetry, electroseparation, controlled current methods, coulometric, potentiometric, and amperometric methods.

References

1. A. J. Bard and L. R. Faulkner, Electrochmical Methods, Fundamentals and applications, John Wiley, 1980.
2. Bockris and Reddy, Electrochemistry, vol 1 & 2, Plenum, 1973.
3. H. Kissinger, Electroanalytical Techniques, John wiley, 1998.

CHE 5005 Green Chemistry

Background, origin and principles of green chemistry. Atom economy and other metrics of greenness. Examples of green processes. Microwave and sonochemical synthesis. Supported catalysts and reagents. Synthesis using enzymes and biocatalysts. Green solvents. Solventless or alternate media conditions: supercritical, fluorous and ionic liquid media. Green chemistry in industries. Green Industrial processes – examples. Sustainable and recyclable resources for chemical industries. Designing for pollution prevention. Designing of biodegradable polymers.

References

1. R. Sanghvi and M. M. Srivastava, "Green Chemistry", Narosa
2. P. T. Anastas and J. C. Warner, "Green Chemistry: Theory and Practice," OUP.

Course Outcome:

- Learning about green chemical industry, including principles and technology.
- Introduction to green and sustainable concepts.

CHE 5006 Industrial Catalysis

Surface area and porosity measurement – measurement of acidity of surfaces; Support materials – preparation and structure of supports – surface properties, preparation of catalysts – introduction of precursor compound – pre-activation treatment – activation process.

General methods of synthesis of zeolites, mechanism of nuclear formation and crystal growth, structures of some selected zeolites – zeolites A, X and Y, pentasils – ZSM-5, ZSM-11, shape selective catalysis by zeolites.

Deactivation of catalysts, classification of catalyst deactivation processes, poisoning of catalysts, coke formation on catalysts, metal deposition on catalysts, sintering of catalysts, Regeneration of deactivated catalysts, feasibility of regeneration, description of coke deposit and kinetics of regeneration.

Basic concepts in phase transfer catalysis – phase transfer catalyzed reactions – basic steps of phase transfer catalysis – effect of reaction variables on transfer and intrinsic rates – outline of compounds used as phase transfer catalysts.

Oil based chemistry; catalytic reforming; catalytic cracking; paraffin cracking; naphthenic cracking; aromatic hydrocarbon cracking; isomerization; hydrotreatment; hydrodesulphurization; hydrocracking; steam cracking; hydrocarbons from synthesis gas; Fisher-Tropsch process, Mobil process for conversion of methanol to gasoline hydrocarbons. Catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources.

References

1. R.B. Anderson, "Experimental methods in catalysis research", Vol I, II, Academic press, NY, 1981.
2. R. Szostak, "Molecular sieves: principles of synthesis and identification", Van Nostrand, NY, 1989.
3. R. Hughes, "Deactivation of catalysts", Academic press, London, 1984.
4. G. Ertl, H. Knozinger and J. Weitkamp, "Handbook of Heterogeneous Catalysis" Vol 1-5, Wiley- VCH, Weinheim, 1997.
5. R.J. Farrauto and C.H. Bartholomew, "Fundamentals of Industrial Catalytic Processes", Blackie Academic and Professional – Chapman and Hall, 1997.
6. R. Pearce and W.R. Patterson, "Catalysis and chemical processes", Academic press, Leonard Hill, London, 1981.
7. C.M. Starks, C.L. Liotta and M. Halpern, "Phase Transfer Catalysis – fundamentals, applications and industrial perspectives", Chapman & Hall, New York, 1994.

Course Outcome:

- Understand the mode of action of catalysts, classification of catalysts and comparison of homogeneous and heterogeneous catalysis.
- Knowledge of methodology in catalyst preparation.
- Knowledge of characterization and evaluation of catalysts.
- Focus on major industrial processes.

CHE 5007 Inorganic Photochemistry

Absorption, excitation, photochemical laws, quantum yield, electronically excited states, life times-measurements of the times. Flash photolysis, energy dissipation by radiative and non-radiative processes, absorption spectra, Frank-Condon principle, photochemical stages-primary and secondary processes.

Excited states of metal complexes: Comparison with organic compounds, electronically excited states of metal complexes, charge transfer spectra, charge transfer excitations.

Photosubstitution, photooxidation and photoreduction, lability and selectivity, zero vibrational levels of ground state and excited state, energy content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states.

Metal complex sensitizer, electron relay, metal colloid systems, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxidereduction.

References

1. A.W. Adamson and P.D. Fleischauer Concepts of Inorganic Photochemistry, Wiley.
2. Inorganic Photochemistry, J. Chem. Educ. vol. 60 No. 10, 1983.
3. S. J. Lippard, Progress in Inorganic Chemistry, Vol. 30^{th} Edn., Wiley.
4. Coordination Chem. Revs. 1981, vol. 39, 121, 1231, 1975, 14, 321, 1990 97, 313.
5. Balzari and V. Carassiti Photochemistry of Coordination Compounds, Academic Press.
6. G. J. Ferraudi, Elements of Inorganic Photochemistry, Wiley.
7. D.M. Roundhill, “Photochemistry and photophysics of Metal complexes”, Springer, Ed., 1994.

CHE5008 Materials Chemistry

Glasses, ceramics, composites and nanomaterials. Preparation, properties and manufacture. Thin films, Langmuir-Blodgett films. Thin film preparation techniques. Properties and application of thin films. Liquid crystals, types and ordering. Optical properties of LCs. Polymeric LCs. Ionic and superconductors. Preparation, characterization and conductance of superconductors. Organic solids. Molecular devices. Conducting organics. NLO materials and data storage materials.

References

1 D. R. Askeland, P. P. Pradeep, The Science & Engineering of Materials, 5thEdn.,, Thomson-Engineering, 2005.

2. H. V. Keer, Principles of solid state, Wiley Eastern.

3. M. Ashby, H. Shercliff and D. Cebon, Materials: engineering, science, processing and design, Butterworth-Heinemann, 2007.

4. M. Wilson, Nanotechnology-Basic Science and Energy Technologies, Taylor & Francis, Inc. 2002.

CHE 5009 Nano Chemistry

Synthesis of nano materials- physical, chemical, biological and hybrid methods. Fullerenes, carbon nanotubes, Nanocomposites and nanofillers: formation, properties.

Analysis of Nano Materials: spectral methods of analysis such as SEM, TEM, X-ray diffraction etc.

Nano-science, types of nanotubes, molecular computers. Lipids, templates, proteins, optical memory and DNA, information and probes, photodynamic therapy.

Applications: molecular electronics. Biomolecular imaging. Photon trapping, nanoholes and photons, formation imaging, solar absorbers, nanostructural polymers, photonic crystals. Nanostructured materials, energy conversion and storage. Semiconductors, transistors, nanofabrication of quantum computers nanomedicines: medical diagnosis, targeted drug delivery. Nanosensors, molecular nanomachines, green in nanoscience, nanomaterial applications in environmental chemistry.

References

1. S.C. Tjong "Nanocrystalline Materials: Their Synthesis-Structure-Property Relationships & Applications", Elsevier Ltd, London, 2006.
2. Jose A. Rodríguez, Marcos Fernández-García "Synthesis, Properties and Applications of Oxide Nanomaterials", John Wiley & Sons, Inc, Canada, 2007.
3. C. Brechignac, P. Houdy, M. Lahmani, "Nanomaterials and Nanochemistry",Springer Berlin Heidelberg, New York, 2007.
4. C. C. Koch, I Lya, A. Ovid'ko, S. Seal and S. Veprek "Structural Nanocrystalline Materials Fundamentals and Applications", Cambridge University Press, Cambridge, 2007.
5. M. Wilson, K. Kanengara, G. Smith, M. Simmons and B. Raguk, Nanotechnology Basic Science and Energy Technologies, Overseas press (I), N.D., 2005.
6. K. J. Klabunde, Nano Materials in Chemistry, John Wiely Sons Inc., 2001.
7. S. K. Kulkarni, Nano Technology Principles and Practices, Capital Publishing Company New Delhi, 2009.

Course Outcome:

- Adequate understanding of the various nanochemistry principles.
- Understanding periodic trends and their relation to the properties of nano materials

CHE 5010 Natural Products Chemistry

Structure of typical terpenoids such as pinene, camphor, hirsutene, abietic acid and squalene. Structure of steroids cholesterol, stigmasterol, estrone, progesterone, testosterone. Chemistry of polyphenolics. Structure determination of representative examples of pyrrolidine, piperidine, indole, 52uinolone, and isoquinoline alkaloids; Structure of beta□-lactam antibiotics –penicillin G.

References

1. K. Nakanishi, Natural Product Chemistry Blackie Publications, 3 Vols.
2. R.H. Thomson, Chemistry of Natural Products – Wiley, New York, 1996.
3. I. L. Finar, Advanced Organic Chemistry, ELBS, New Delhi, 1975.

CHE 5011 Polymer Chemistry

Macromolecules and polymers. Types of polymers. Degree of polymerization. Polymerization processes and their kinetics and mechanisms. Free radical, cationic and anionic, step Growth polymerization. Linear and cyclic, group Transfer, metathesis and ring opening polymerizations. Copolymerization. Gelation and Cross linking. Polymerization techniques. Bulk Solution, melt, suspension, emulsion and dispersion techniques. Coordination polymerization.

Living polymers.

Configuration and conformation, Tacticity. Stereo regular polymers. Polymer Characterization. Molecular weights and its distribution. Methods for determining molecular weights. Glassy and Rubbery States.

Methods for polymer structure determination. Structure-property relationship. Elastomeric and viscoelastic states. Rubbery elasticity. Degree of cross linking Polymer structure-property relationship, crystalline and amorphous structure. Introduction to polymer additives, blends and composites.

Industrial and specialty polymers: polyethylene, polypropylene, polystyrene, PVC, PVA, PAN, PA, PMMA and related polymers. Copolymers. Reaction polymers. Polyamides, polyesters. Epoxides, polyurethanes, polycarbonates, phenolics, PEEK, Silicone polymers. Reactions of polymers. Polymers as aids in Organic Synthesis. Polymeric Reagents, Catalysts, Substrates, Liquid Crystalline polymers. Conducting polymers.

References

1. F.W. Billmayer, "Textbook of Polymer Science", 3rdEdn., Wiley. N.Y. 1991.
2. J.M.G. Cowie, "Polymers: Physics and Chemistry of Modern Materials:, Blackie. London, 1992.
3. P.J. Flory, "A Text Book of Polymer Science", Cornell University Press. Ithacka, 1953.
4. J. R. Fried, "Polymer Science and Technology", Prentice Hall of India.
5. C. E. Carraher Jr, "Polymer Chemistry", 6thEdn., Marcel Dekker, Inc.

CHE 5012 Supramolecular Chemistry

Molecular recognition, Non-covalent interactions. Self-assembly. Cation receptors: crown ethers, cryptands, spherands, calixarens. Anion receptors. Neutral receptors. Clathrates, cavitands, cyclodextrins, cyclophanes. Supramolecular reactivity and catalysis. Supramolecular devices. Supramolecular assemblies in biological systems. Photosynthesis, Oxygen transport, Biomimetics.

References

1. J. M. Lehn, Supramolecular Chemistry, Concepts and Perspectives, VCH, 1995.
2. H. Dodziuk, Introduction to Supramolecular Chemistry, Kluwer Academic, 2002.
3. F. Vogtle, Supramolecular Chemistry, An Introduction, John Wiley & Sons, 1991.
4. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, A Concise Introduction, John Wiley, 2000.
5. A. Bianchi, K. B. James, E. G. Espana, Supramolecular Chemistry of Anions, Wiley-VCH, 1997.
6. M. Fujita, Molecular Self-assembly Organic Versus Inorganic Approaches, Springer, 2000.

CHE 5013 Renewable Energy

Energy: Past, Today, and Future. A brief history of energy consumption. Energy &environment, non-renewable energies. Energy and power concepts, hydroelectricity principles and basic concepts of other conventional energy resources. Solar energy: radiation, solar flux and angles, solar thermal collectors, passive solar cells, solar photo-voltaic based on crystalline and amorphous silicon and other materials (polymers, organic & inorganic molecules). Wind energy: wind resources, wind turbines, turbine generator systems. Ocean energy: wave & tides characteristics and statistics, wave energy devices, ocean biomass. Bioenergy and biofuels, geothermal resources, geothermal technologies.

References:

1. Godfrey Boyle, "Renewable Energy, Power for a sustainable future", 2004, Oxford University.
2. Aldo V. da Rosa, "Fundamentals of Renewable Energy Processes", 2005, Academic Press.
3. K. Kalyanasundaram, Dye-sensitized Solar Cells, 2010, EPFL Press, Switzerland.
4. C. S. Solanki, Solar Photovoltaics: Fundamentals Technologies and Applications, 2011, 2nd Edition, PHI Learning.

CHE 5014 Crystallography

X-ray crystallography, solids, crystalline and amorphous solids, Crystal lattice, unit cell and asymmetric unit. Crystal systems and Bravais lattice. Weiss indices, Miller indices and Miller planes. X-ray diffraction by crystals, Bragg's law, Diffraction patterns and reciprocal lattice. Symmetry elements, inversion centre, reflection, rotation, rotation-inversion. Screw axis, Glide planes. Space groups, Herman-Mauguin notation. Space groups, Space group diagrams. Special positions in space groups. Centrosymmetric and non-centrosymmetric space groups. Systematic absences in crystal data. Structure factors. Structure solution, phase problem, direct methods, Patterson methods. Refinement, least square method. Constraints and restraints. Hydrogen bonding and π-π interactions.

References

1. Li-ling Ooi, 2010, Principles of X-ray Crystallography, Oxford University press
2. Gregory S. Girolami, X-ray Crystallography, University Science books, California

Course Outcome:

- Recognition of crystalline structures and symmetry classes, space groups etc. and formulation of models of crystalline structures.
- Understanding the properties and symmetry of crystals.
- Learning about the basic aspects of X-ray diffraction and crystal structure analysis.

CHE 5015 Pharmaceutical Chemistry

Bond type and bond strength, Hydrocarbons: alkanes, alkenes, aromatic and alkylhalides, Amines, Neutral and acidic nitrogen compounds, Oxygen- and sulphur-containing functional groups

Protein structure and its relevance to drug action, DNA structure and its importance to drug action, Drug absorption, distribution, metabolism and excretion.

Structure, activity and drug design, Drugs affecting the adrenergic system, Drugs exerting non-adrenergic effects on cardiac output and vascular tone, Drugs interacting with mammalian enzymes

Central nervous system depressants, Analgesics, Local anaesthetics, Anticholinergic agents, Antihistamine drugs, CNS stimulants and CNS-active drugs affecting the serotonergic system, Drugs affecting the endocrine system

Anticancer drugs, Antimicrobial chemotherapy, Antiviral drugs, Antifungal chemotherapy, Antiparasitic drugs, Vitamins and minerals, Biotechnologically produced products, Drug and gene delivery systems, The tonic and toxic effects of alcohol and its metabolites

References

Pharmaceutical Chemistry, Edited by David G Watson BSc PhD PGCE Reader in Pharmaceutical Sciences, Strathclyde Institute of Pharmacy and Biomedical Sciences, School of Pharmacy, University of Strathclyde, Glasgow, UK, Churchill Livingstone, Elsevier 2011

CHE 5016 Molecular Fluorescence and Applications

Basics of Molecular Fluorescence:

Fundamental laws of photochemistry, nature of light and matter, Interaction of light with matter, Mechanism of absorption and emission, electronic transitions, selection rules, spectroscopic term symbols, physical properties of electronically excited molecules, Jablonski diagram, photophysical properties of the electronically excited molecules. Photophysical kinetics of bimolecular processes. Electron and energy transfer reactions.

Principles of steady-state and time-resolved fluorometric techniques:

Steady-state spectrofluorometry: Operating principles of a spectrofluorometer, Correction of excitation spectra, Correction of emission spectra, Measurement of fluorescence quantum yields, Problems in steady-state fluorescence measurements,

Time-resolved fluorometry: General principles of pulse and phase-modulation fluorometries, Single-photon timing technique and measuring fluorescence lifetimes.

Resonance energy transfer and its applications:

Determination of distances at a supramolecular level using RET, Single distance between donor and acceptor, Distributions of distances in donor–acceptor pairs and RET in ensembles of donors and acceptors etc. Effect of polarity on fluorescence emission and Polarity probes: What is polarity? Empirical scales of solvent polarity based on solvatochromic shifts, Single-parameter approach, Theory of solvatochromic shifts, Examples of PCT fluorescent probes for polarity and effects of specific interactions.

Fluorescent molecular sensors of ions and molecules:

Fundamental aspects, pH sensing by means of fluorescent indicators, Fluorescent molecular sensors of cations, Fluorescent molecular sensors of anions, Fluorescent molecular sensors of neutral molecules and surfactants

References

1. *Fundamental of Photochemistry* - KK Rohatgi Mukherjee, New Age Publishers; Third edition, ISBN-10: 8122434320.
2. *Molecular Fluorescence Principles and Applications* - Bernard Valeur, Wiley-VCH Verlag GmbH ISBNs: 3-527-29919-X (Hardcover); 3-527-60024-8 (Electronic).
3. *Principles of Fluorescence Spectroscopy* - Joseph R. Lakowicz, Springer Publishers, 3rd edition, ISBN 978-0-387-46312-4.

CHE 5017: Physical Principles of Chemical Engineering

Stoichiometric principles – material and energy balances. Fluid flow – Bernoullis equation and its applications – pipes and fittings – Industrial pumps – flow through.

Fouriers law – simple numerical problems on conduction – natural and forced convection – heat transfer equipment –Drying - Different types of dryers-Distillation –vapour liquid equilibria –distillation methods – continuous rectification of binary systems – design method for theoretical plates – HETP concepts.

Adsorption and adsorption principles, Extraction–liquid extraction–ternary diagram–selection of solvent, Crystallization – types of crystallization equipment – material and energy balances.

Laws of crushing, types of crushers and grinders – settling, floatation and filtration concepts.

Nitration, sulphonation, halogenation, esterification, amination, saponification andhydrogenation, role of the above unit processes in such industries as petroleum,drugs, pharmaceuticals and organic synthesis

REFERENCES

1. W.I.Badger and I.T.Banchero Introduction to Chemical Engineering, McGraw Hill Book co., Inc., Kogakusha, 1988.
2. P.H.Groggins, Unit Processes in Organic Synthesis, McGraw Hill Book Co., Kogakusha, 1984.
3. J.H.Perry, Handbook of Chemical Engineers, McGraw Hill Book Co.2002.

Course Outcome:

Physical Principles of Chemical Engineering covers the basic introductions and understanding of principles of chemical engineering. This course could expose the preliminary outstanding to M.Sc chemistry students to work in chemical industries. As there are opportunities for M.Sc chemistry students in chemical industries, such base introduction and awareness might help them in finding job in chemical industries.

CHE 5000V Industrial/Academic Visit

Credits: Non-credit course

Preferably at the end of third semester/beginning of the fourth semester, the students shall be taken to the either industries or academic universities/institutes (or may be both) to disseminate the importance of chemistry. Students shall be accompanied by minimum two faculty members during the visit. The faculty members shall ensure that the importance of the chemical/material processes (such as petrochemical or petroleum, pharmaceutical, catalyst manufacture, polymer technology, rubber technology, flourochemical, refinery processes, API development etc.) are being explained by the industry/company representative during the visit (if not the faculty shall explain before/during the visit and may be connected with theory taught in class.

Students shall be taken to the academic universities/institutes of national importance where there are adequate instrumentation facilities are available. During the visit the students shall be shown and explained all the characterization/analysis techniques such as NMR, HRMS, X-diffraction, optical, scanning and electron microscopy techniques, electronic and emission spectroscopy, thermal analysis etc.

Thirty contact hours are essential for passing this course

Evaluation: At the end of the visit, students are required to submit a detailed report of the visit based on which the accompanied faculty members shall award grade.

Course Outcome:

- Exposure of students to a few chemical/material processes carried out in industries/companies.
- Students will be familiarized with latest characterization/analysis techniques and help inculcate scientific thrust towards basic and applied research.
- This course helps to improve observing, thinking, interpreting and predicting skills of the students