Department of Chemistry

The Department of Chemistry under the School of Physical and Chemical Sciences forms a key component of the university. The department is composed of dynamic faculty members and research scholars who are actively engaged in knowledge creation and dissemination at the frontiers of the Chemical Sciences. The discipline has an encompassing effect on the biological and physical sciences and therefore considered a central science. Knowledge and skills in chemistry play a crucial role in finding the solutions to most of the challenges (eg. energy, disease, environment) faced by the mankind today. The department believes in interdisciplinary approach of learning and fosters a culture of excellence. Undergraduate students of chemistry have been nurtured and mentored well to compete at the national and international level (eg. selection for the summer research fellowships of National Academies of Sciences, award at National Science Film Festival and more…). The postgraduate programme is being started with this new academic session in 2018. The department envisage scaling greater heights with the launch of post-graduate programmes and producing globally competent chemists who can solve the pressing problems of the nation.

MSc. Programme in Chemistry

The programme is for the students who have an interest in chemistry and a desire to explore the frontiers of science. This is a unique programme that combines core chemistry (Organic, Inorganic and Physical) with Nano Chemistry and Green Chemistry. Alongwith thorough grounding in chemistry, it equips the students with the knowledge and skills in the emerging interdisciplinary area of green nanotechnology which has now become a crucial requirement for the sustainable development globally. Computational Chemistry and Medicinal Chemistry have also been incorporated to equip the students better. The programme envisages creating good bench strength of future scientists who can solve a wide range of issues and contribute to the scientific advancement of the nation.

There is ample opportunities and employability of chemists having sound knowledge, analytical skills and hand-on training on the sophisticated instruments. The chemical industry is India's one of the largest manufacturing sectors and plays an integral role in the country's economic development. The Indian chemical sector currently accounts for 13-14% of total exports. In terms of volume of production, it is the twelfth-largest in the world and the third-largest in Asia. Currently, the per capita consumption of products of the Indian chemical industry is one-tenth of the world average, which reflects the huge potential for further growth. The "Make in India" scheme has further given a fresh impetus to this sector. For a sustainable, environment-friendly growth, the sector is looking for new technologies that incorporate green chemistry and nanotechnology and there lies the exciting and excellent career opportunities for young chemists. Besides chemical industry, the training imparted in the interdisciplinary area of green nanotechnology will also enable the students to diversify and join other sectors such as energy, photovoltaics, photonics, biosensing and healthcare etc.

The curriculum has been designed to keep abreast with changing times. In the long run, the programme is likely to produce globally competent chemists with bright innovative ideas. By understanding the nuances of chemistry, these young scientists would be creating new tools, products and technologies to address some of the world's biggest challenges such as (just to name a few) clean affordable energy, biomedical devices and drugs for treating diseases, biosensing and environmental remediation etc.

- **DURATION OF THE PROGRAMME:** Four semesters, July – December (odd semesters) and January – May (even semesters).
- **ADMISSION PROCEDURE:** The admission to the course shall be through an entrance examination, Central University Common Entrance Test (CUCET-2018) to be conducted on all-India basis.

- **ELIGIBILITY OF THE CANDIDATES:**
  Candidates who have passed B.Sc. examination of any recognized university or its equivalent examination with minimum of 55% marks in aggregate (or in honours subject) (50% in the case of SC/ST students) and who have taken Chemistry (General/Honours) as one of the subjects at the third year of the B.Sc.
- **Credit System: Theory**: 01 hour lecture per week – 01 credit.
  Experimental Chemistry & Computational Chemistry: 02 hours – 01 credit
- **Distribution of Points:** Theory (T) = 100 points; Practical (P) = 100 points.

Theory of each paper: 100 points
Distribution of points (Theory):

1A: Continuous Assessment Test (CAT): 3 CATs will be conducted at regular interval in the entire semester in regular class hour to access student's progress. Each CAT will carry 10 points. Total 3 x 10 = 30 Points.

1B: End-Term: 70 points.

Experimental Chemistry Lab.: 100 points
Distribution of points (Practical): Tentative

1A: Class Participation/involvement in experiment/cleanniness/skill: 10 points

2B: Distribution of points of Final Exam: (i) Exam: 40 points, (ii) Viva: 30 points, (iii) Overall record (Performance, write-up and on time submission throughout the semester): 20 points.]

- **Grading System:**

There will be 10-point Scale Grading System starting with 4 and ending at 10. There will be additional Grade 'F' with Grade Point 'Zero'. A student having received Grade 'F' in a course will have to reappear in the examination of the said course. The following grading system will be used:

Letter Grade	**Numerical Grade Point**	**Class Interval (in %)**
O (Outstanding)	10	Above 90 and ≤ 100
A+ (Excellent)	9	Above 80 and ≤ 90
A (Very Good)	8	Above 70 and ≤ 80
B+ (Good)	7	Above 60 and ≤ 70
B (Above Average)	6	Above 50 and ≤ 60
C (Average)	5	Above 45 and ≤ 50
P (Pass)	4.5	40 to 45
F (Fail)	0	< 40
Ab (Absent)	0	Absent

Note:

(i) F= Fail, and the students graded with 'F' in a Programme or Course shall be required to re-appear in the examination.

(ii) The minimum qualifying points for a course shall be 4.5 (i.e., 'P' grade).

(iii) The students shall have to qualify in the Continuous Internal Assessment and the End-Semester examinations taking together.

Salient features of the programme

- Nano Chemistry, Green Chemistry, Medicinal Chemistry and Agrochemistry have been incorporated in the curriculum to develop a thorough understanding of these emerging fields and their relevance in daily life of mankind.
- Computational Chemistry, theory and labs, have also been made part of the curriculum to make the students proficient in theoretical modeling and simulations.
- Besides imparting in-depth knowledge, hands-on training will also be given to students on sophisticated instruments which are a prerequisite for being employable in industries and succeed in cutting edge research.
- For proper utilization of summer break period, students will be encouraged to take up a summer activity. This activity may include research internship in academic/research institutions or industrial lab. It may also include activities related to science communication such as writing a popular science article in a magazine or writing a review article in a scientific journal. It also includes activities such as science film making etc. The summer project should be done at the end of 2nd Semester during the summer break period.
- Students from both PCB and PCM streams can join this degree programme. We believe that knowledge of both mathematics and biology is necessary to understand the nuances of chemistry. The students having mathematics background may opt for the basic biology course while the students having biology background may opt for basic mathematics course in the first semester.
  - The M.Sc. Programme in Chemistry follows CBCS approach.
  - A minimum of 96 credits has to be completed by the students during the entire programme. However, students can earn more credits by opting for additional courses from the elective baskets. The mximum credit to be earned this way is limited to 104.
  - Out of the 96 credits a total of 56 credits should be earned through core courses. For semester 1st and 3rd, students have to choose courses from odd semester courses list. Similarly, for semester 2nd and 4th, students have to choose courses from even semester courses list.
  - Out of the 96 credits a total of 40 credits should be earned through electives following cafeteria model under CBCS scheme. Out of 40 credits, 8 credits (two courses) should be earned through elective courses offered by other departments/centres/SWAYAM.
  - Students can opt one or more courses (Core as well as elective, minimum 4 credits) from SWAYAM portal in consultation with the faculty members/mentors of the department.
  - The department will announce in advance about the elective courses to be run in the coming semester.
  - For 1st and 3rd semesters, students have to choose courses from the list of core and elective courses to be run in the odd semesters. Similarly, for 2nd and 4th semesters, students have to courses from the list of core and elective courses to be run in the even semesters
  - Core and elective courses of the department are of 4 credits each.
  - Students will not be allowed to repeat the elective courses during the programme.
  - A student can opt for more than one elective in one semester.
  - *Out of elective courses offered, only few selected ones will be floated in a particular academic session and at least a certain number (to be decided by the departmental committee) of total students enrolled must opt for a particular elective paper to run that course*.
  - Allotment of different branches of specialization will be done at the end of second semester. An order of preference has to be submitted by each student for the three different specializations. Based on the two parameters, the choice and performance upto 2nd semester, the specialization will be allotted subject to maximum of 40% of total strength of students in one specialization
  - Students may earn 24 credits or more in each semester. However, the total credits earned during the entire programme should not exceed 104.

COURSE STRUCTURE

(Minimum Core/Electives Credits = 56/40)

FIRST SEMESTER (ODD SEMESTER)

Code No.	Title	Theory/Practical (Hrs/Week)	Total Marks	Credits
MSCHE1001C04	Group Theory, Bonding and Metal-Ligand Equilibrium	4	100	4
MSCHE1002C04	Bonding, Stereochemistry and Reaction Mechanism (I)	4	100	4
MSCHE1003C04	Basic Concepts of Physical Chemistry	4	100	4
MSCHE1004C04	Inorganic Chemistry Lab	8	100	4
Departmental Elective	**One** or more courses to be selected from the elective basket for odd semesters	4	100	4
Open Elective (Inter-School or Inter-Department or SWAYAM elective)	**One** or more courses to be selected from the elective basket for odd semester	4	100	4

SECOND SEMESTER (EVEN SEMESTER)

Code No.	Title	Theory/Practical (Hrs/Week)	Total Marks	Credits
MSCHE2001C04	Photochemical and magnetic properties of complexes and nuclear chemistry	4	100	4
MSCHE2002C04	Reaction Mechanism (II), Pericyclic and Photochemical Reactions	4	100	4
MSCHE2003C04	Quantum Mechanics and Statistical Thermodynamics	4	100	4
MSCHE2004C04	Physical Chemistry Lab	8	100	4
Departmental Elective	**Two** or more courses to be selected from the elective basket for even semesters	4	100	4

THIRD SEMESTER (ODD SEMESTER)

Code No.	Title	Theory/Practical (Hrs/Week)	Total Marks	Credits
MSCHE3001C04	Carbohydrates, Hetrocyclic Compounds, Organometallic Reagents and Synthetic	4	100	4
MSCHE3002C04	Project-I and Scientific Activities	-	100	2+ 2 = 4
MSCHE3003C04	Organic Chemistry Lab	8	100	4
Departmental Elective	**Two** or more courses to be selected from the elective basket for odd semesters	4	100	4
Open Elective (Inter-School or Inter-Department or SWAYAM elective)	**One** or more courses to be selected from the elective basket for odd	4	100	4

FOURTH SEMESTER (EVEN SEMESTER)

(Common to students of all branches)

Code No.	Title	Theory/Practical (Hrs/Week)	Total Marks	Credits
Chemistry Specialisaton				
MSCHE4001C12	Project-II	-	100	12
Departmental Elective	**Three** or more courses to be selected from the elective basket for even semesters	4	100	4

ELECTIVES COURSES

(Minimum 40 Credits[#])

Code No.	Title of the Paper	Teaching/contact Hrs/week	Total Marks	Credits
Elective-Basket for 1st Semester (Odd Semester)				
• **At least one elective has to be choosen.**				
MSCHE1001E04	Supramolecular Chemistry	4	100	4
MSCHE1002E04	Chemistry of Biomolecules	4	100	4
MSCHE1003E04	Green Chemistry I: Solvents & Synthesis	4	100	4
SWAYAM Elective* [#] Few courses have to be taken from SWAYAM portal and from other schools/departments Students will also be encouraged to take a self study/skill-based course available on SWAYAM portal. No credit will be awarded for this as it would be a zero-credit course. * SWAYAM Courses will be reviewed and announced by the department periodically.				
Elective-Basket for 2nd Semester (Even Semester)				
• **At least two electives have to be chosen.**				

MSCHE2001E04	Solid State and Structural Chemistry	4	100	4
MSCHE2002E04	Advanced Instrumental Techniques-I	4	100	4
MSCHE2003E04	Green Chemistry II: Catalysis	4	100	4
MSCHE2004E04	Nucleoside, Advances in Nucleic Acid and Proteins	4	100	4
MSCHE2005E04	Chemistry of Natural Products	4	100	4
Elective-Basket for 3rd Semester (Odd Semester)				
• **At least two electives have to be chosen.**				
MSCHE3001E04	Atom Dynamics in Solid and Advanced Magnetochemistry	4	100	4
MSCHE3002E04	Surface Phenomena, Chemical Dynamics and Spectroscopy	4	100	4
MSCHE3003E04	Chemistry of Materials	4	100	4
MSCHE3004E04	Advanced Photochemistry	4	100	4
MSCHE3005E04	Medicine and Agrochemicals	4	100	4
MSCHE3006E04	Nano Chemistry	4	100	4
Elective-Basket for 4th Semester (Even Semester)				
• **At least three electives have to be chosen.**				
MSCHE4001E04	Reaction mechanism, Organometallics and Advanced Bioinorganic Chemistry	4	100	4
MSCHE4002E04	Applications of spectroscopy techniques to inorganic systems	4	100	4
MSCHE4003E04	Advanced Inorganic Materials	3 (L)+2 (P) = 5	100	3+1 = 4
MSCHE4004E04	Dynamic Stereochemistry, reagents and Retrosynthtic analysis	4	100	4
MSCHE4005E04	Medicinal, combinatorial and Organomettalic reagents in Organic synthesis	4	100	4
MSCHE4006E04	Spectroscopy and catalysis in Organic synthesis	3 (L)+2 (P) = 5	100	3+1 = 4
MSCHE4007E04	Advanced Quantum Mechanics and Surface Chemistry	4	100	4
MSCHE4008E04	Applied Electrochemistrty	4	100	4
MSCHE4009E04	Lasers in Chemistry	4	100	4
MSCHE4010E04	Green Energy Systems	4	100	4
MSCHE4011E04	Advanced Instrumental Techniques-II	4	100	4

FIRST SEMESTER (ODD SEMESTER)

Course Details			
Course Title: Group Theory, Bonding and Metal-Ligand Equilibrium			
Course Code	**MSCHE1001C04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		
Assessment and Evaluation	• 30% - Continuous Internal Assessment (Formative in nature but also contributing to the final grades) • 70% - End Term External Examination (University Examination)		

Course Objectives

- To develop understanding of group theory and apply the concepts of symmetry to molecular systems
- To enhance the understanding of ionic and covalent bonding in view of point groups and molecular symmetry.
- To impart in-depth knowledge about metal-ligand equilibrium reactions
- To equip the students with necessary skills to determine the equilibrium constants using various instrumental techniques

Learning Outcomes: After completion of the course the learners will be able to:

- Identify the symmetry elements present in a molecule,
- Assign the pint groups to a molecule and perform symmetry operations
- Analyze the molecular structure and bonding in molecules and coordination complexes with the help of group theory
- Determine the overall and stepwise formation constants of metal-complexes

UNIT- I

Chemical Bonding:VSEPR model, shapes of molecules-ClF_3, ICl_4^-, TeF_5^-, I_3^-, $TeCl_6^{2-}$, XeF_6, $SbCl_6^{3-}$, IF_7, ReF_7, XeF_8^{2-}, TaF_8^{3-}, Bent rules and energetics of hybridization; electronegativity and partial ionic character; Bonds- Multicenter, Synergic and Agostic bonding.
Lattice energy: Born-Lande equation, Kapustinskii equation; polarizability and partial covalent character, radius-ratio rules, structures of simple solids, Zintl- isoelectronic relationship in solids. Molecular orbital theory: LCAO and MO diagrams of heteronuclear diatomic (CO, NO, HF, ICl) and triatomic molecules (CO_2 and NO_2^-).

UNIT- II

Metal-ligand bonding- Stereoisomerism- coordination numbers 3 to 8. Crystal field theory, salient features, spectro chemical series, splitting of d-orbitals in tetragonal, square planar, trigonal bipyramidal and square-pyramidal geometry, applications of CFT- colours of transition metal complexes, magnetic properties of octahedral complex, distortion of octahedral complex, CFSE and their uses, factors affecting CFSE, limitations of CFT, experimental evidence for metal-ligand covalent bonding in complexes, nephelauxetic effect, Ligand Field Theory, MO theory: tetrahedral and octahedral complexes (including π- bonding), angular overlap model. Stereochemical non-rigidity, self-assembly in supramolecular chemistry.

Boding in metal clusters: M-M bond and metal atom clusters, carbonyl and halide clusters, bonding in $[ReCl_8]^{2-}$. Metal carbonyl clusters- LNCC's and HNCC's. Electron counting in carbonyl clusters, Wades-Mingos and Lauher rules.

UNIT-III

Metal-Ligand equilibria in solution- Step-wise and overall formation constant and their relationship, trends in step-wise constant, kinetic and thermodynamic stability of metal complexes, factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate effect, macrocyclic effect and their thermodynamic origin. Determination of binary formation constant by Ph- metry, spectrophotometry, polarography and ion exchange methods.

Structure and bonding- Structure and bonding in isocyanide, CO, NO, N_2 tertiary phosphine and other similar ligands and their transition metal complexes.

Stereoisomerism- Chirality, optical activity and isomerism in inorganic complexes.

UNIT-IV

Symmetry and Group Theory in Chemistry: Definition of groups, subgroups, cyclic groups, conjugate relationships, classes, simple theorems in group theory. Symmetry elements and symmetry operations, point groups, Schöenflies notations, representations of groups by matrices, reducible and irreducible representations, characters of representations, Great Orthogonality Theorem (without tproof) and its applications, character tables and their uses (representations for the C_n, C_{nv}, C_{nh}, D_{nh} etc groups to be worked out explicitly) Mulliken symbols for irreducible representations Direct products.
Unifying principles: Interaction of electromagnetic radiation with matter- time-dependent perturbation theory, transition moment integral, selection rules- symmetry and spin forbidden transitions.

SUGGESTED TEXT BOOKS

1. Basic Inorganic Chemistry- F. A. Cotton, G. Wilkinson and P. L. Gaus; John Wiley and sons. Inc, 6th edition.
2. Advanced Inorganic Chemistry, 6th edition; F. A. Cotton and G. Wilkinson.
3. Inorganic Chemistry; J. E. Huheey, E. A. Keiter and R. L. Keiter, Addison; Wesley.
4. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford, ELBS; Oxford University Press.
5. Chemistry of Elements; N. N. Greenwood a n d A. E. Earnshaw, Butterworth Heinemann (1997).
6. Concise Inorganic Chemistry, 5th edition; J. D. Lee (1996).
7. Inorganic Chemistry, 3rd Edition; Gary. L. Miessler and Donald. A. Tarr (2007).
8. Chemical Applications of Group Theory, F. A. Cotton, Wiley Eastern (1976).
9. Molecular Symmetry, D. S. Schonland, Van Nostrand (1965).

SUGGESTED REFERENCE BOOKS

1. Basic Organometallic Chemistry: Concepts, Syntheses and Applications of Transition metals, 2010, CRC Press and Universities Press.

Course Details			
Course Title: Bonding, Stereochemistry and Reaction Mechanism (I)			
Course Code	**MSCHE1002C04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives: To learn the basic and advanced concepts of chemical bonding, aromaticity and reaction mechanism. Develope knowledge in-depth about different kinds of addition reaction. Recognise the characteristic of free radicals, its mechanism and application in organic synthesis.

Learning Outcomes: Students will be able to make the correlation of bonding, structure, reactivity and stability of organic molecules. And by using above concepts, students will be able to understand the spatial arrangements of substituents in organic molecules and their implication in selectivity in reaction. Here students will know the depth knowledge of different kinds of reaction and mechanism and also know different tools available to predict the reaction mechanism.

UNIT-I

Nature of Bonding in Organic Molecules-Molecular orbital theory, Delocalized chemical bonding: Conjugation, cross conjugation, resonance, Aromaticity, Aromatic systems, Antiaromaticity, Homo-aromaticity. Alternant and non-alternant hydrocarbons.

Physical Organic Chemistry: Classification of reactions and mechanisms. Thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates.

Methods of determining mechanisms: Based on the structure of products, determination of the presence of intermediates, isotopic labelling, isotope effects, from stereochemical evidence.

Effect of structure on reactivity:- Resonance and field effects; steric effects. The Hammett equation and linear free energy relationship, substituent and reaction constants, physical significance and use of Hammett plot.

UNIT-II

Stereochemistry-: Chirality in compounds with a stereogenic centre, Stereogenic unit: Center of chirality, axis of chirality, plane of chirality and helicity. Stereochemistry of allenes, alkylidene, biphenyls, cyclophanes, and ansa compounds, *trans*-cyclooctene, helicenes, benzphenanthrenes and spiranes (with a stereogenic axis).

Conformational analysis: Conformational analysis of cycloalkanes: cyclobutane, cyclopentane, cychexanes (monosubstituted e.g., methyl, *iso*-propyl, *tert*-butyl and di-substituted cyclohexanes e.g., dialkyl, dihalo, diols) and cycloheptane.

Nomenclature and conformations of fused rings *eg* indane, decalines and perhydrophenanthrene and bridged ring systems like bicyclo[2.2.2], [2.2.1] systems.

UNIT-III

Addition Reactions: Addition to carbon-carbon multiple bonds: mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals. Regio, stereo- and chemoselectivities. Cis and trans additions. Orientation and reactivity. Addition to cyclopropane ring. Additions to C=C double bonds that are related to cycloadditions and form three-membered rings. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Addition of alkenes and/or alkynes to alkenes and/or alkynes. Ene synthesis. Michael reaction.

Addition to carbon-heteroatom multiple bonds: Mechanism of metal hydride reduction (NaH, LiH, $LiAlH_4$, and $NaBH_4$) of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents and organolithium reagents to carbonyl compounds and unsaturated carbonyl compounds. Conversion of aldehydes to nitriles. Hydrolysis of nitriles and addition of amines to isocyanates. Formation of xanthates. Wittig, Mannich and Stobbe reactions.

UNIT-IV

Reactive Intermediates and their chemistry: Generation, structure, stability and reactivity of carbocations, carbanions, carbon free radicals, carbenes and nitrenes, benzyne.
Free radical reactions: Free-radical mechanisms in general. Free-radical substitution mechanisms. Mechanisms at an aromatic substrate. Neighboring group assistance in free-radical reactions. Halogenation at an alkyl carbon and an allylic carbon, Gomberg-Bachmann reaction, Meerwein arylation, Sandmeyer reaction, Kolbe reaction and Hunsdiecker reaction.
Reactions and application of carbenes.

SUGGESTED TEXT BOOKS

1. Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley (2008).
2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg Plenum, (1990).
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman, (2000).
4. Structure and mechanism of Organic Chemistry, C. K. Ingold, Cornell University Press (1999).
5. Organic Chemistry, R. T. Morrison and R N Boyd, Prentice-Hall, (1998).
6. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackie Academic and Professional, (1996).
7. Stereochemistry of Organic Compounds, D. Nasipuri, New-Age International, (1999).
8. Stereochemistry of Carbon Compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley, (1994).
9. Organic Chemistry, Volumes I and II, I L Finar, Longman, (1999).

SUGGESTED REFERENCE BOOKS

1. Mechanism and Theory in Organic Chemistry, T. H. Lowry and K. S. Richardson, Addison-Wesley, 1998.

Course Details			
Course Title: Basic Concept of Physical Chemistry			
Course Code	**MSCHE1003C04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives: To lay the foundations of quantum mechanics by giving the mathematical background and concept of operators.

- To make the students understand the significance of wavefunction and discuss various types of quantum confinements, particle in a 1-D box etc.
- To develop an understanding of thermodynamics and apply the concepts to various physicochemical processes and systems
- To equip the students with necessary skills to analyse physicochemicalchanges with the help of phase diagrams
- To develop an undwestanding of chemical kinetics
- To acquaint the students with the core concepts of electrochemistry

Learning Outcomes: After completion of the course the learners will be able to:

- Analyse a given siuation from quantum mechanical viewpoint and write appropriate Schrodinger equation
- Explain physicochemical changes with the help of phase diagrams
- Find out the rate and order of reations

- Use electrochemical techniques for estimation of metal ions and biologically rlev
- Design a photoelectrochemical cell

UNIT-I

Mathematical Concepts: Logarithmic relations, curve sketching, linear graphs and calculation of slopes, differentiation of functions like f(x), e^x, x^n, sin x, log x; maxima and minima, partial differentiation and reciprocity relations. Integration of some useful/relevant functions, permutations and combinations, Factorials and Probability.

Quantum Mechanics-I: Introduction to quantum mechanics. Schrödinger wave equation. Time-independent and time-dependent Schrödinger wave equations and the relation between their solutions. Eigenfunctions and Eigenvalues. Physical Interpretation of wave function.

Concepts of Operators: Laplacian, Hamiltonian, Linear and Hermition operators. Angular Momentum operators and their properties. Commutation of operators. Normalization, orthogonality and orthonormality of wave functions. Average (expectation) values. Postulates of quantum mechanics. Solutions of Schrödinger wave equation for a free particle, particle in a ring, particle in a three-dimensional box. Quantum mechanical degeneracy, tunnelling (no derivation). Application of Schrödinger equation to harmonic oscillator, rigid rotator. Eigenfunctions and eigenvalues of angular momentum. Ladder operator method for angular momentum.

UNIT-II

Thermodynamics-I

Thermodynamics: Concepts of partial molar properties – partial molar free energy, chemical potential, partial molar volume and its significance. Gibbs-Duhem equation, Gibbs-Duhem-Margulus equation. Determination of partial molar volume: Graphical method, intercept method and apparent molar volume method. Concept of fugacity; Determination of fugacity by graphical method and compressibility factor method. Activity and activity coefficient: Determination of activity coefficient by EMF and solubility method. Thermodynamics of non-ideal system-Excess thermodynamic function, $G^{E,}$ ^{SE}, H^E etc.

Phase Rule: Derivation of phase rule from the concept of chemical potential. Application of Phase Rule to three components system: Principle of triangular diagram: Plots for a mixture of three liquids consisting of one, two and three pairs of partially miscible liquids.

UNIT-III

Chemical Dynamics-I: Macroscopic and microscopic kinetics, Review of theories of reaction kinetics, Collision theory and Transition state theory, Comparison of collision theory with transition state theory, Arrhenious equation- characteristics, Significance of energy of activation, Temperature coefficient and its evaluation. Thermodynamical formulation of reaction rates (Wyne-jones and Eyring treatment), Reaction between ions in solutions – Influence of ionic strength on reaction rates (primary and secondary salt effects).
Concept of Steady state kinetics, Chain reactions – chain length and chain inhibition, comparison of photochemical and thermal reactions, Mechanisms of thermal and photochemical reactions between hydrogen-bromine and hydrogen-chlorine. Comparative study of thermal and photochemical hydrogen-halogen reactions. Pyrolysis of acetaldehyde, Decomposition of ethane.

UNIT-IV

Electrochemistry-I

Electrochemistry of solutions: Ionic atmosphere, Debye-Huckel theory for the problem of activity coefficient, Debye-Huckel limiting Law, its modification for finite size of ions and for appreciable concentration, Debye-Hückel-Onsagar conductance equation and its extension to short-range ion-ion interaction leading to ion pair formation (Fuss modification). Bjerrum's model for pair-wise ionic association, Ion association, triple-ion pairs, and conductance minima. Thermodynamics of electrified interface, derivation of electro capillary

Lipmann's equation, surface excess, thermodynamic aspects of surface excess. The method of determination and measurement of interfacial tension as a function of applied potential difference across the interface.

SUGGESTED TEXT BOOKS

1. Physical Chemistry: A Molecular Approach, McQuarie and Simon, Viva, New Delhi, (2001).
2. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill, (1988).
3. Quantum Chemistry, Ira. N. Levine, Prentice Hall, New Jersey, (1991).
4. Quantum Chemistry, R. K. Prasad, New Age International, 2nd edition, (2000).
5. Chemical Kinetics- K. J. Laidler, McGraw Hill. Inc. New York (1988).
6. Principles of Chemical Kinetics – House J. E. Wm C Brown Publisher, Boston, (1997).
7. Kinetics and Mechanism–A. A. Frost and R. G. Pearson, John-Wiley, New York, (1961).
8. Chemical Kinetic Methods – C. Kalidas, New Age International Publisher, New Delhi, (1995)
9. S.H. Maran and C. F. Pruton, 4th Edn. Oxford & IBH publishing Co. Pvt. Ltd. New Delhi (1965).
10. Physical Chemistry- P. Atkins and J. D. Paula, 9th Edn. Oxford University Press (2010).
11. Modern Electrochemistry Vol-1 and 2 J. O'M Bockris and A. K. N. Raddy, Plenum NewYork (1978).
12. Text book of physical chemistry Samuel Glastone, 2nd edition, Mac Millan India Ltd (1991).
13. Principles and applications of Electrochemistry- D. R. Crow 3rd edition Chapmanhall London (1988).
14. A Textbook of physical Chemistry Vol-2, 3 and 5- K. L. Kapoor 5th edition Mcgraw Higher Ed (2015)

SUGGESTED REFERENCE BOOKS

1. Kinetics and Mechanism of Chemical Transformations- J. Rajaraman and J. Kuriakose, Mc Millan. (1986).
2. Biological Chemistry by James P Allen, Wiley-Blackwell, 2008.
3. Introduction to Biophysical Chemistry, R. Bruce Martin, McGraw-Hill, NY, 1964.
4. Physical Chemistry with applications to Biological systems, Ramond Chnag, Mc Millan publishing Co.inc, New York 1977.
5. Computational Chemistry, Introduction to Theory and Application of Molecular and Quantum Mechanics by Errol Lewars, Springer 2016.
6. Molecular Modelling: Principle and Application, 2nd Ed. by Andrew R. Leach, Addison-Wesley Longman Ltd. 2009.

Course Details			
Course Title: Inorganic Chemistry Lab			
Course Code	**MSCHE1004C04**	**Credits**	4
L + T + P	0 + 0 + 4	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	120 Hours
Methods of Content Interaction	Lecture, Reagents Preparation and Practical Classes		

OBJECTIVE:

- To make students proficient in qualitative analysis of acidic and basic radicals including rare ones such as W,Zr, U, Ce, Mo etc
- To impart effective training in synthesis of inorganic complexes and its characterization using various instrumental techniques such as UV-Vis-NIR absorption and luminescnece spectroscopy, FTIR spectroscopy, TG/DTA analysis etc.
- To equip the students with necessary skills in quantitative analysis

Learning Outcomes

After completion of the course the learners will be able to:

- Find the cations and anions present in a given sample

- Synthesize inorganic complexes of various types and characterize it using instrumental techniques
- Determine, quantitatively, the amount of metals present in an ore, alloy or solution

Lab-I: Qualitative Abalysis

Semi micro qualitative analysis of mixtures containing one anion, one common cation and one less familiar element: W, Mo, Ce, Th, Zr, V, U and Li.

Lab-II: Synthesis and characterization of inorganic complexes

Preparation and quantitative analysis of inorganic complexes:

1. Cis- and trans- potassium dioxalatodiaquachromium(III) complex [analysis of oxalate and chromium]
2. Hexamminecobalt(III)chloride [analysis of cobalt]

Lab-III: Quantitative analysis of metals in alloys, ores and solution

Gravimetric analysis

1. Gravimetric determination of Fe in iron ore as Fe_2O_3.
2. Gravimetric determination of Ni in Cu and Ni solution.
3. Gravimetric determination of Fe in Fe and Cr solution.

Volumetric analysis

1. Volumetric estimation of Ca and Mg in Dolomite solution.
2. Volumetric estimation of Cu in Cu and Ni (German silver).
3. Volumetric estimation of Fe in Cu and Fe solution.

SECOND SEMESTER (EVEN SEMESTER)

Course Details			
Course Title: Photochemical and magnetic properties of complexes and nuclear chemistry			
Course Code	**MSCHE2001C04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To make students understand the structure and properties of inorganic chains, rings and sheets
- To equip the students with necessary skills in electronic spectroscopy of metal complexes
- To acquaint the students with the photochemical reactions of coordination compounds
- To introduce the core concepts of magnetochemistry for analysing properties of complexes
- To develop an understanding of nuclear and rdaiochemistry

Learning Outcomes: After completion of the course the learners will be able to:

- Analyse the optical/electronic spectra of coordination compounds
- Make use of the photochemical behaviour of complexes in designing solar cells and other applications.
- Design and perform photochemical reactions of metalcomplexes
- Analys the magnetic properties of complexes
- Explain the various phenomena taking place in the nucleus
- Understand the working of nuclear reactors
- Utilize various nuclear techniques for analytical and biomedical applications

UNIT-I

Chemistry of main group elements- Structure and bonding in boranes, carboranes, metallocarboranes, Wade's rules, borazines, phosphazenes, S, N- compounds.
Silicates-Classification, structures, isomorphous replacement, pyroxenes, layeredandvitreous silicates, zeolites and molecularsieves.

UNIT-II

Electronic spectra of coordination compounds- Spectroscopic ground states, selection rules, term symbols for d^n ions, Racah parameters, Orgel, Correlation and Tanaube-Sugano diagrams, spectra of 3d metal-aqua complexes of trivalent V, Cr, divalent Mn, Co and Ni, $CoCl_4$, calculation of Dq, B and β parameters, CT spectra. Spectral properties of Lanthanide and Actinide metal complexes.

UNIT-III

Magnetic properties of coordination compounds- Types of magnetic behaviour, magnetic susceptibility and its determination- Gouy, Faraday, VSM method. Diamagnetic correction, orbital contribution, spin-orbital coupling, ferro- and antiferromagnetic coupling, spin-crossover. Magnetic properties of Lanthanide and Actinide metal complexes.
Photochemical reactions of transition metals complexes: Basic photochemical processes, Kasha's rule, quantum yield, Jabolnskii diagrams, photo substitution reactions, photo-redox reactions, ligand photoreactions, photoreactions and solar energy conversion.

UNIT-IV

Nuclear Chemistry-The atomic nucleus-elementary particles, quarks, classification of nuclides based on Z and N values, nuclear stability, nuclear potential, binding energy. Nuclear Models: Shell model-salient features, Nuclear reactions: Q value, cross sections fission and fusion, fission products and fission yields; Radioactivity: Radioactive decay and equilibrium, theories of α, β-, β+ and γ-decay, internal conversion, Auger effect, Bremmstrahlung, counting techniques such as G.M. ionization and proportional counter. Radiation dosimetry and radiation protection, Chemical effects of nuclear transformations; 'Hot-atom' chemistry
Applications of radioactivity: Radioactive techniques; tracer technique, Neutron Activation Analysis (NAA), Radioimmunoassay, Boron-Neutron Capture Therapy (BNCT), Positron Emission Tomography(PET), Proton-induced X-ray Emission (PIXE), Therapeutic uses of Gamma-rays.

SUGGESTED TEXT BOOKS

1. Basic Inorganic Chemistry- F. A. Cotton, G. Wilkinson and P. L. Gaus; John Wiley and sons. Inc, 2007.
2. Chemistry of elements- N. N. Greenwood and A. E. Earnshaw, Butterworth Heinemann (1997).
3. Inorganic Chemistry IV edition; J. E. Huheey, E. A. Keiter and R. L. Keiter, Addison; Wesley, 2008.
4. Inorganic Chemistry, III edition, D. F. Shriver, P. W. Atkins and C. H. Langford, ELBS; Oxford University Press, 1999.
5. Inorganic Electronic spectroscopy, A. B. P. Lever, Elsevier. (1968).
6. Magnetochemistry, R.L. Carlin, Springer Verlag, 1986.
7. Electronic Absorption Spectroscopy and related Techniques, D. N. Sathyanarayana, University Press (2001).
8. Inorganic Chemistry a Unified Approach by W. W. Porterfield, Elsevier 2005 2nd edition.
9. Textbook of inorganic chemistry by G. S. Sodhi, Viva books Pvt. Ltd (2011).
10. Essentials of nuclear chemistry, 4th edition; H. J. Arniker, NAIL publishers (1995);
11. Nuclear and Radioactive chemistry; Friedlander, Kennedy and Miller; Chapters 8 and 9, 1981.

Course Details			
Course Title: Reaction Mechanism (II), Pericyclic And Photochemical Reactions			
Course Code	**MSCHE2002C04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

OBJECTIVE: To develop the concept in depths about reaction mechanism related to substitution, addition, elimination and rearrangement reaction. To develop the concept in depths about reaction mechanism related to substitution, elimination and rearrangement reaction. To give idea about photochemical process/reaction and its application in organic synthesis. To develop and use the concept of pericyclic reaction.

Learning Outcomes: After completion of the course the learners will be able to:

- Here students will know the depth knowledge of substitution, elimination, rearrangement reactions and their role in organic synthesis.
- Students will able to understand the unique photochemical process and their role in organic synthesis
- Students will be able to get knowledge of pericyclic reactions, their mechanism and use in synthesis of different kinds of organic molecules.

UNIT-I

Substitution Reactions

Aliphatic and aromatic Electrophilic Substitution Reactions: The arenium ion mechanism. Orientation and reactivity. Energy profile diagrams. The *ortho*/*para* ratio, *ipso* attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Effect of leaving group.

Substitution at allylic carbon (allylic rearrangement), at a trigonal carbon (hydrolysis of esters and amides), substitution at a vinylic carbon. Neighboring group participation and S_Ni reactions, non-classical carbonium ion.

Aliphatic and Aromatic Nucleophilic substitution reactions: The S_NAr, S_N1, benzyne and SR_N1mechanisms. Reactivity: effect of substrate structure, leaving group and attacking nucleophile. Goldberg reaction, Bucherer reaction, Schiemann reaction, von Richter reaction, Sommelet-Hauser and Smiles rearrangements.

S_E2, S_E1 and S_Ei mechanisms. Hydrogen exchange, migration of double bonds, α- halogenation of aldehydes, ketones and acids. Aliphatic diazonium coupling, nitrosation at carbon bearing active hydrogens, diazo transfer reaction, decarboxylation of aliphatic acids, haloform reaction, Haller-Bauer reaction.

UNIT-II

Elimination Reactions: The E_2, E_1 and E_1cB mechanisms. Orientation of the double bond. Reactivity-effects of substrate structure, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination reactions (including Chugaev reaction).

Rearrangements: General Mechanistic considerations-nature of migration, migratory aptitude, memory effects. Wagner-Meerwein, Pinacol-Pinacolone, Fries, Wolff, Beckmann, Hofmann, Curtius, Lossen and Schmidt rearrangements. Benzil-benzilic acid rearrangement, Arndt-Eistert reaction, Tiffeneau- Demjanov reaction, Firtsch-Buttenberg-Wiechell rearrangement. Stevens, Wittig and Favorskii rearrangements, Dienone-phenol, Baker-Venkatraman rearrangement. Baeyer-Villiger oxidation. Neber rearrangement. Benzidine rearrangement.

UNIT-III

Photochemistry: Physical and Chemical processes, Jablonski diagram. Photosensitization, quantum efficiency, quantum and chemical yields, solvent effects, Stern-Volmer plot, delayed fluorescence etc.

Photochemistry of functional groups:

(A) Olefins: Cis-trans isomerism, [2 + 2]-cycloaddition, rearrangements. Reaction of conjugated olefins; di-methane rearrangements (including oxa- and aza- di--methane rearrangements).

(B) Ketones: Excited state of C=O. Norrish type-I and type-II cleavages. Paterno-Buchi reaction. -unsaturated ketones. [2+2] addition. Rearrangement of cyclohexadienones (application in the synthesis of some important natural products).

(C) Aromatic compounds: Photorearrangement of benzene and its derivatives, cycloaddition of benzene.

(D) Photochemical oxidations and reductions: Cycloaddition of singlet molecular oxygen {[2+2], [4+2]-additions}. Oxidative coupling of aromatic compounds, photoreduction by hydrogen abstraction

UNIT-IV

Pericyclic reactions Molecular orbital symmetry, Woodward-Hoffmann correlation diagrams. FMO and PMO approaches. Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Electrocyclic reactions: conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems.

Cycloadditions: antarafacial and suprafacial additions, $[\pi m_s + \pi n_a]$ and $[\pi m_s + \pi n_s]$-cycloadditions. $[\omega 2_a + \pi 2_s]$ and $[\pi 4_s + \omega 2_s]$-cheletropic reactions. Regio, enantio and Endo selectivities in Diels-Alder reactions. Hetero Diels-Alder reaction.

Sigmatropic rearrangements: suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties. [*i, j*]- sigmatropic rearrangements (including Walk, Claisen, Cope, oxy and aza-Cope rearrangements), Ene reaction

SUGGESTED TEXTBOOKS

1. Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley (2008).
2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Volume A and B, 2008.
3. A Guide Book to Mechanism of Organic Chemistry, Peter Sykes, Longman (2000).
4. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall (1998).
5. Principles of Organic Synthesis, ROC Norman and J. M. Coxon, Blackie Academic and Professional, 2012.
6. Stereochemistry of Organic Compounds, D. Nasipuri, New-Age International (1999).
7. Stereochemistry of Carbon Compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley (1994).
8. Organic Chemistry, Volumes I and II, I L Finar, Longman. (1999).

SUGGESTED REFERENCEBOOKS

1. Frontier Orbitals and Organic Chemical Reactions, I. Fleming, Wiley, London, 1976.
2. Pericyclic Reactions- A text Book, S. Sankararaman, Wiley VCH, 200
3. Organic Photochemistry, J. M. Cozen and B. Halton, Cambridge University Press (I st Edition) 1974

Course Details			
Course Title: Quantum Mechanics and Statistical Thermodynamics			
Course Code	**MSCHE2003C04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To equip the students with the skills in quantum mechanics
- To develop a comprehensive understanding of statistical thermodynamics.

Learning Outcomes: After completion of the course the learners will be able to:

- Formualate and solve quantum mechanical equations for a givn system
- Apply concepts of statistical thermodynamics to various systems

UNIT-I

Quantum Mechanics-II: Schrödinger equation to hydrogen atom in spherical polar co-ordinates. Solution of Φ , Θ equation and statements of solution of R equation. Total wave functions of hydrogen atom. Quantum numbers and their characteristics. List of wave functions for few initial states of hydrogen like atoms. Diagrams of radial and angular wave functions. Radial and angular distribution function and their significance. Electron spin (Stern-Gerlach experiment), spin- orbital, anti-symmetry and Pauli-exclusion principle, Slater determinants. Coupling of angular momenta. Russell-Saunders and JJ-coupling, Term symbols. Spin-orbital interaction and explanation of term multiplicities (Na-D doublet). Zeeman effect.

UNIT-II

Approximate methods: Need for approximate methods. Perturbation method. Rayleigh Schrödinger perturbation theory for time-independent non-degenerate system. Application to electron in a box under the influence of an electric field. Application to He atom. Variation theory-statement and proof. Application of variation method to particle in a one-dimensional box and He atom.

UNIT-III

Thermodynamics-II

Statistical Thermodynamics: Introduction: Concept of ensembles, partition functions and distributions, microcanonical, canonical and grand canonical ensembles, canonical and grand canonical partition functions, Boltzmann, Fermi-Dirac and Bose-Einstein distributions. Gibbs paradox and Sackur – Tetrode equation. Concept of thermal wavelength. Molecular partition functions – transitional, rotational, vibrational, electronic, nuclear. Equipartition theorem and its validity. Problems and their Solutions. System of interacting molecules – Imperfect gas. Specific heat of electron gas, Bose condensation.

UNIT-IV

Non-equilibrium Thermodynamics: Thermodynamic criteria for non-equilibrium states-Phenomenological Laws and Onsager's Reciprocity relations, Coupled and Non-coupled reactions, Entropy production and entropy flow. Electro-kinetic Phenomenon.

Introductory Computational Chemistry: Introduction about the computational chemistry and molecular modelling, Coordinate systems, Concept of 2D and 3D structure, molecules, Surfaces, Molecular energetic profile, Brief idea about the computational softwares for drawing, visualization and simulation of small and large molecules. Basic concept of Chemoinformatics, 3D-Structure file system and Databases

SUGGESTED TEXT BOOKS

1. Introduction to Quantum Mechanics, David J Griffiths 2nd edition Cambridge University Press (2017).
2. Quantum Chemistry, Donald McQuarrie, 2nd edition, University Science Books (2007).
3. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill, (1988).
4. Quantum Chemistry, Ira. N. Levine, Prentice Hall, New Jersey, (1991).
5. Quantum Mechanics, John Powell and Bernd Crasemann, 1st edition Narosa Publishing House (1998).
6. D. A. McQuarrie, Statistical Mechanics, University Science Books, California (2005).
7. D. Chandler, Introduction to Modern Statistical Mechanics, Oxford University Press, 1987.
8. A Textbook of physical Chemistry Vol- 4 and 5, K. L. Kapoor 5th edition Mcgraw Higher Ed (2015).
9. Thermodynamics, by Rajaraman and Kuriacose, East-West Press, (1986).
10. Statistical Thermodynamics, M. C. Gupta (Wiley Eastern Ltd.) 1993.
11. Elementary Statistical Thermodynamics, N. D. Smith, Plenum Press, NY, (1982).
12. Elements of Classical and Statistical Thermodynamics, L. K. Nash, Addison-Wiley (1979).
13. Thermodynamics, Statistical Thermodynamics and Kinetics by Thomas Engel & Philip Reid, Pearson Education inc. (2007).

SUGGESTED REFERENCE BOOKS

1. P. Atkins and J. Paula, Physical Chemistry, 8th Edition, Oxford University Press, Oxford, 2006.
2. R. S. Berry, S. A. Rice and J. Ross, Physical Chemistry, 2nd Edition, Oxford University Press, Oxford 2007.
3. B. Widom, Statistical Mechanics-A Concise Introduction for Chemists, Cambridge University Press, 2002.

Course Details			
Course Title: Physical Chemistry Lab			
Course Code	**MSCHE2004C04**	**Credits**	4
L + T + P	0 + 0 + 4	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	120 Hours
Methods of Content Interaction	Lecture, Reagents Preparation and Practical Class		

Course Objectives

To equip the students with necessary laboratory skills for performing experiments of chemical kinetics snad catalysis

- To acquaint students with basics of computational chemistry and molecular modelling
- To make the students proficient in drawing stereochemical structure of a molecules using software tools such as ChemDraw, ChemOffice
- To impart training to the students in various instrumental techniques such as conductometry, potentiometry, UV-Vis spectrophotometry, FTIR spectroscopy and cyclic voltamtery.
- To make students learn how to perform qualitative and quantitative analysis using such equipment.

Learning Outcomes: After completion of the course the learners will be able to:

- Determine the activation energy, rate constant and equilibrium constant of different reactions using various instrumental techniques.

Lab -I

1. Comparison of acid strength (HCl and H_2SO_4) by studying acid-catalysed hydrolysis of methyl acetate at lab temperature.
2. Determination of rate constant and energy of activation for the base hydrolysis of ethyl acetate Verification of Beer's Law for Cu^{2+} and Fe^{2+} ions
4. Estimation of Fe^{2+} ions concentration in the given solution by titration of FAS versus $KMnO4$ through colorimetric method.
5. Estimation of Fe^{2+} ions concentration using EDTA through colorimetric method
6. Phase diagram of two component systems and determination of E_C, E_T and the determination of the composition of given unknown.
7. Determination of partial molar volume of solute –H_2O system by apparent molar volume method.
8. Determination of the viscosity of a mixture by apparent molar volume method.
9. Verification of Freundlich and Langmuir isotherms for adsorption of oxalic/acetic acid on activated charcoal.

Lab-II

1. Computer Fundamentals (Operating Systems e.g. MSDOS, Windows, LINUX).
2. Introduction and application about the computational chemistry & molecular modelling software.
3. Understanding of the chemical structure and physico-chemical properties using chemistry software "ChemOffice Ultra"
   a) Draw a chemical structure and reactions with the example of organic and inorganic substances along with physical notations such as bonding, enthalpy, entropy, etc.
   b) Concept, application and handling of 2D & 3D structure. Draw the structures of biological active molecules.
4. Understand the concept of stereochemistry and draw the stereochemical structure by using the example of nucleoside and amino acid.
5. Minimization of the chemical structure with the example of nucleoside.
6. Compute the structural and physico-chemical properties (e.g.; bond length, bond angle, dihedral angle, conformation, partial charge, steric energy, etc.) of the target molecule using ChemDraw Tools.

Lab-III

1. Study the hydrolysis of methyl acetate at two different concentrations of HCl and report the relative strength.
2. Determination of dissociation constant of a given indicator by colorimetric method.
3. Study of kinetics of autocatalytic reaction between KMnO4 versus oxalic acid.
4. Determination of degree of hydrolysis of aniline hydrochloride at room temperature and calculation of dissociation constant of the base by pH metry
5. Study of variation of viscosity of a liquid with temperature, determine the constant A and B.
6. Analysis of a binary mixture of two miscible liquids and to determine the composition of the given unknown mixture.
7. Evaluation of Arrehenius parameter for the reaction between K2S2O8 versus KI (first order)

Lab -IV

Conductometry

1. Conductometric titration of strong acid with string base
2. Conductometric titration of weak acid with string base
3. Conductometric titration of oxalic acid with string base
4. Conductometric titration of acid mixture with string base
5. Conductometric titration of $AgNO_3$ with KCl
6. Conductometric titration of $BaCl_2$ with Na_2SO_4
7. Determination of Molar and Equivalent conductivity of a given strong electrolyte (and weak electrolyte) as a function of concentration

Potentiometry

8. Determination of strength of HCl, CH3COOH and oxalic acid versus NaOH by pH metry
9. To determine the acidic and basic dissociation constant of an amino acid and determination of isoelectric point by pH metry.
10. Determination of dissociation constant of H3PO4 using potentiometric/pHmetric method.
11. Determination of strength of Fe^{2+} solution by performing potentiometric titration with K2Cr2O7 or KMnO4
12. pH-metric titration of mixture of weak and strong acid against NaOH
13. Determination of stability constant of copper-ethylenediamine complex by potentiometry
14. Determination of pka of amino acids by potentiometric titration

Additional experiments based on cyclic voltamtery and electrogravimetry

15. Estimation of copper by electrogravimetric method
16. Polarographic analysis, identification and estimation of metal ions (Pb2+, Cd2+, Zn2+)
17. Cyclic voltammetry of a standard redox couple (ferricyanide-ferrocyanide couple)

SUGGESTED BOOKS

1. Practicals in Physical Chemistry, P S Sindhu, Macmillan, 2005
2. Practical Physical Chemistry, Alexander Findlay, CHIZINE PUBN, 2018
3. Experimental Physical Chemistry: A Laboratory Textbook, Arthur Halpern, George McBane, 1. W. H. Freeman, 2006
4. Experiments in Physical Chemistry: Second Revised and Enlarged Edition, J. M. Wilson, R. J. Newcombe, A. R. Denaro, Elsevier, 2016
5. Experimental Physical Chemistry - Scholar's Choice Edition, Daniels Farrington, Scholar's Choice, 2015
6. Quantitative Chemical Analysis, 9th edition, Daniel C. Harris, W. H. Freeman, 2015
7. Vogels Textbook Of Quantitative Chemical Analysis, Mendham, Pearson Education India, 2006

THIRD SEMESTER (ODD SEMESTER)

Course Details			
Course Title: Carbohydrates, Hetrocyclic Compounds, Organometallic Reagents and Synthetic Methods			
Course Code	**MSCHE3001C04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

OBJECTIVE: To impart knowledge about natural products like carbohudrates and protein and know the significance in biochemistry and drug developments. Develope understandings about hetrocyclic compounds and explore orgamometallic reagents for organic reactions. Finally buildup a different tools available for functional group transformations.

Learning Outcomes: Students will be able to

- Describe/recognize the structure of mono-, di-, and polysaccharides, describe their physical and chemical properties and their function in living organisms. Predict the products of chemical reactions of carbohydrates (acetal/hemiacetal formation or oxidation). Describe what happens during carbohydrate digestion, glycolysis, glycogenesis, and glycogenolysis.
- Describe/recognize amino acid structures, describe their physical and chemical properties, and predict how their ionic charges change with pH. Define primary, secondary, tertiary and quaternary structure in proteins and identify the types of interactions important in each case.
- This course aims at providing theoretical understanding of heterocyclic chemistry which includes various methods for ring synthesis and application of those methods for the preparation of specific groups of heterocyclic systems. The students will be made familiar with particular properties, reactions, and applications of the most important as well as less common heterocycles.
- Students will be able to develope a basic knowledge of organomettalic compounds and their application in organic synthesis.

UNIT-I

Carbohydrates: Introduction, classification and nomenclature. Configuration of monosaccharides. Erythro and threo- diastereomers. Chemical reactions, interconversions in carbohydrates: glucose to fructose, aldopentose to aldohexose and aldohexose to aldopentose, epimerization, Determination of the ring size of monosaccharide. Mechanism of mutarotation.

Disaccharides and polysaccharides: sucrose, Lactose, cellobiose, Reducing and non-reducing sugars, Polysaccharide: Starch, glycogen, Cellulose and Chitin, analysis of carbohydrates.

Amino Sugars: Synthesis of amino sugars (β-D- Glucosamine, galactosamine, N-acetylmuramic acid (NAMA), N-acetyl neuraminic acid NANA). C- and N- glycosides. Synthesis of aldonic, uronic, aldaric acids and alditols. Photosynthesis of carbohydrates.

Significance of carbohydrates in biochemistry, drug discovery and natural product synthesis as a chiron approach.

UNIT-II

Heterocyclic compounds: Brief introduction of hetrocyclic compounds. Nomenclature of heterocyclic compounds. Structure, reactivity, synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyrimidine, purine and indole.

Benzo-fused heterocycles: Synthesis and reactions of benzofurans, benzothiophenes, benzoxazoles, benzothiazoles and benzimidazoles. Six-membered heterocycles with two or more heteroatoms: Synthesis of Diazines and triazines.

UNIT-III

Organometallic complexes- Stability and decomposition pathways, classification of ligands, nomenclature of organometallic complexes, 16 and 18 electron rules. Electron counting- covalent and ionic models.

Synthesis, structure, bonding and reactivity of the following organotransition metal complexes: Carbenes, carbynes, alkenes, alkynes, allyl moieties, butadiene, cyclobutadiene, cyclopentadiene, arenes, cycloheptadienyl moieties and cyclooctatetraene moieties. Ring slippage reactions, cyclometallation reaction.

Organometallic compounds of main group elements- General Trends, structure and bonding in Li and Al alkyls.

Fluxional behaviour in organometallic complexes: Fluxionality and dynamic equilibria in complexes containing CO, η^2-olefin η^3-allyl and dienyl complexes, η^5-complexes.

Organometallic compounds in organic synthesis: Green rules, synthesis and use of Zinc dialkyls, Collman's reagent, Metal carbonyls in organic synthesis, Pauson Khand reaction, Heck reaction, Suzuki reaction, Stille coupling, Kumada coupling, Negishi coupling, Sonogashira reaction, Tebbe reagent, hydrozirconation

UNIT-IV

Methods in Organic Synthesis: A review of various synthetic methods in organic chemistry: Formation of C-C, C=C, C≡C, C-X, C=X bonds and various rings (namely 3, 4, 5, 6, 7 and 8-membered ring); chemo selective synthesis, Selected syntheses of natural and unnatural products having these ring systems. Introduction of domino, tandem reaction, multicomponent reaction, click chemistry and metathesis reaction with a detailed discussion, Principles of use of ultrasound and microwave in organic synthesis.

Modern Synthetic Methods: Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction and Ugi reaction. Brook rearrangement; Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reactions, directed ortho metalation.

SUGGESTED TEXT BOOKS

1. Warren S. Organic Synthesis: The Disconnection Approach, Wiley.
2. Smith M. B. and March J. March's Advanced Organic Chemistry, Wiley.
3. Carey F. A. and Sundberg R. Advanced Organic Chemistry, Part B, Plenum Press.
4. Trost B. M. and Fleming I. Comprehensive Organic Synthesis, Pergamon Press.
5. Norman R. O. C. and Coxon J. M. Principles of Organic Synthesis, Nelson Thornes
6. Strategic applications of named reactions in organic synthesis, Kurti L. and Czako B., Academic Press, 2005
7. Joule, J. A. and Mills, K. Heterocyclic Chemistry, Fifth Edition, Wiley, 2010.
8. Gilchrist, T. L., Heterocyclic Chemistry, Prentice Hall, 1997.
9. Acheson, R. M. An Introduction to the Chemistry of Heterocyclic Compounds, 3rd Ed, Wiley India Pvt Ltd, 2008.
10. Eicher, T.; and Hauptmann, S.; The chemistry of Heterocycles, Wiley-VCH, Weinheim, 2003.
11. The Organic Chemistry of Sugars, D. E. Levy, P. Fugedi, CRC.

SUGGESTED REFERENCE BOOKS

1. Schlosser, M., Organometalllics in Synthesis, A manual, John Wiley, New York, 1996.
2. Hegedus, L.S.; Transition metals in the synthesis of complex organic molecules, second edition, University Science, Book, CA, 1999.
3. Astruc, D.; Organometallic Chemistry and Catalysis, Springer Verlag, 2007.
4. Davies, S. G.; Organotransition metal chemistry: Applications to organic synthesis, Pergamon Press, New York, 1986.
5. Organic Synthesis with Carbohydrates, G. J. Boons, K. J. Hale, Blackwell.

Course Details			
Course Title: Project-I and Scientific Activities			
Course Code	**MSCHE3002C04**	**Credits**	4
L + T + P	0 + 0 + 4	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	
Methods of Content Interaction	(a) Literature Survey, Seminar, Presentation and Viva (b) Scientific activities at societal interface (under Unnat Bharat, Swachh Bharat or any such govt-announced schemes)		

(a) Candidate will be given a research topic during the first week of semester III. The candidate is expected to carry out literature survey, read research articles, make a comprehensive review and give a seminar presentation where they have to show their understanding on the subject and suggest some alternative solution to problems. Seminar presentation and group viva/defence will be conducted at the end of semester III.

(b) Students will be assigned a task which may involve field work and collecting data. The students will then suggest scientific solutions to the problem and the ways to implement them. This work has to be carried out at societal interface under the government-announced schemes such as Swachh Bharat, Unnat Bharat, Samrt Cities, etc. At the end of the work, student will submit a report and give a presentation based on which evaluation will be done.

Course Details			
Course Title: Organic Chemistry Lab			
Course Code	**MSCHE3003C04**	**Credits**	4
L + T + P	0 + 0 + 4	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	120 Hours
Methods of Content Interaction	Lecture, Reagents Preparation, Practicals		

OBJECTIVE: To develop skills of synthesis, purifications and characterisation of organic compounds.

Organic Chemistry Practical-I: Preparation (one stage)

1. Cannizarro reaction: Benzaldehyde.
2. Fries rearrangement: Phenyl acetate.
3. Friedel-Crafts reaction: Benzene and Acetyl chloride.
4. Sandmeyer reaction: 4-Chlorotoluene from 4-toluidine.
5. Oxidation of Cyclohexanol.

6. Preparation of S- Benzylisothiuronium chloride.
7. Synthesis of *p*-iodonitrobenzene
8. Synthesis of N-Phenyl-2,4-dinitroaniline.
9. Synthesis of 2,4,6-tribromoaniline.
10. Synthesis of 2,4-dichlorophenoxyacetic acid.

Purification of above compounds (products) by –crystallization, fractional crystallization, distillation, fractional distillation, vacuum distillation and column chromatography. Use of TLC for identification of Organic compounds.

Organic Chemistry Practical-II

Small scale organic synthesis using some of the following reactions:

i. Acetylation reaction
ii. Oxidations and reductions
iii. Nucleophilic aromatic/aliphatic substitution
iv. Bromination and bromine addition
v. Condensations
vi. Diazotisation reactions

Organic Chemistry Practical-III: Simple Instrumental techniques in Organic Chemistry

1. Determination of specific rotation of given compounds and of racaemic mixture
2. Determination of pka of amino acids by potentiometric titration
3. Estimation of a common drug (paraacetamol) by UV spectroscopy
4. Estimation of Keto-enol tautomerism by IR,
5. Separation of amino acids by thin layer chromatography
6. Separation of proteins by gel electrophoresis
7. Estimation of protein in food samples
8. Estimation of Vitamin A in food samples
9. Determination of concentration of chiral compounds

SUGGESTED TEXT BOOKS

1. A Text Book of Quantitative Inorganic Analysis: A. I. Vogel, 1989.
2. Vogel A. I. *Practical Organic Chemistry*, Longman Group Ltd.
3. Bansal R. K. *Laboratory Manual of Organic Chemistry*, Wiley-Eastern.
4. Ahluwalia V. K. and Aggarwal R. *Comprehensive practical organic chemistry*, University press.
5. Nad A. K.; Mahapatra B. and Ghoshal A. *An advanced course in practical chemistry*, New Central Book Agency (P) Ltd.
6. Wilson, John H. Block, Ole Gisvold, John Marlowe Beale, 2004.

SEMESTER IV (EVEN SEMESTER)

Course Details			
Course Title: Project-II			
Course Code	**MSCHE4001C12**	**Credits**	12
L + T + P	0+ 0 + 12	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	
Methods of Content Interaction	Project Work (including experiments, dissertation, presentation, and viva)		

OBJECTIVE: To introduce students to research in various areas of chemistry by engaging them to carry out a project under the supervision of a faculty for two semesters during the third and fourth semesters.

Candidate will be given a topic of project at the beginning of Semester II. The candidate is expected to collect relevant literature and make a presentation based on the literature and the proposed plan of work at the end of Semester III and it is expected from the students to start their project work during summer vacation or from the first day of semester IV.

CHY- E#– ELECTIVES

Course Details			
Course Title: Supramolecular Chemistry			
Course Code	**MSCHE1001E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To acquaint students with the basic principles of supramolecular chemistry
- To impart knowledge and skills in sythesis of supramolecular structures
- To introduce the concept of self-assembly and its mechanistic aspects
- To make students aware of biomedical and device applications of supramolecular structures

Learning Outcomes: After completion of the course the learners will be able to:

- Explain the binding interactions in supramolecular structures
- Write the synthesis scheme and structures of crown ethers, host-guest compounds
- Apply the concept of 'self-assembly' to make supramoleculars structures
- Discuss the relevance of supramolecular structures in daily life and its applications in molecular devices, medicine and catalysis.

Unit I: Intermolecular interactions

Definition of supramolecular chemistry. Nature of binding interactions in supramolecular structures: ion-ion, Ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p, and van der Waals interactions.

Unit II: Synthesis of suparamolecular structures

Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands., Host Guest interactions, preorganization and complimentarity, lock and key analogy. Binding of cationic, anionic, ion pair and neutral guest molecules. Crystal engineering: role of H-bonding and other weak interactions.

Unit III: Self assembly

Self-assembly molecules: design, synthesis and properties of the molecules, self-assembling by H-bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots.

Unit IV: Applications and recent developments

Molecular devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic.

Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis etc. Examples of recent developments in supramolecular chemistry from current literature

SUGGESTED TEXT BOOKS

1. Supramolecular Chemistry- Concepts and Perspectives (Wiley-VCH, 1995), J.-M.Lehn.
2. Bioorganic, Bioinorganic and Supramolecular Chemistry, P. S. Kalsi and J. P. Kalsi. New Age International Publishers.

SUGGESTED REFERENCE BOOKS

1. P. D. Beer, P. A. Gale, D. K. Smith; Supramolecular Chemistry (Oxford University Press, 1999).
2. J. W. Steed and J. L. Atwood; Supramolecular Chemistry (Wiley, 2000).

Course Details			
Course Title: Chemistry of Biomolecules			
Course Code	**MSCHE1002E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

OBJECTIVE: Acquire foundational knowledge of the chemistry of life. Examine the relationship between the structure and function of biological molecules. And apply this knowledge in research and development in the area of Biomedical Analysis as well as Biomedical Methods and Technology.

UNIT I

Amino acids and Peptide: Amino acids, structural features, optical activity, essential and non-essential amino acids, iso-electric point, synthesis and chemical properties of α amino acids. Peptides: Structure and synthesis, Protecting and activating groups, solid phase peptide synthesis.

Proteins: classifications, primary, secondary, tertiary and quaternary structure of proteins, glycoproteins, denaturation and foldin

Enzyme: Nomenclature and classification, Remarkable properties of enzymes like catalytic power, specificity and regulation, Proximity effects and molecular adaptation, Chemical and biological catalysis. Mechanism of enzyme action: Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors affinity labeling and enzyme modification by site directed mutagenesis.

Receptors: Type of receptors, Receptor-ligand interaction, Enzymes, agonists, partial agonist, inverse agonists, neutral antagonists and antagonist

UNIT II

Coenzyme: Cofactors as derived from vitamins, coenzymes, prosthetic groups, and apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate pyridoxal phosphate, NAD+, NADP+, FMN, FAD, Lipoic acid, vitamin B12. Mechanisms of reactions catalyzed by the above cofactors.

Nucleosides, Nucleotides and Nucleic Acids: Nucleosides, Nucleotides, Elementary idea of nucleic acids and complementary base pairing, ATP: The Carrier of Chemical Energy, Phosphodiester bonds, Oligonucleotides and polynucleotides, Nucleic acids, Secondary and tertiary structures, the double helix

Lipids: Classification and biological importance of fatty acids and lipids, stereochemical notation in lipids, chemical synthesis of phospholipids and glycolipids, properties of lipid aggregates, micelles, bilayers, lyposomes and biological membranes.

UNIT III

Concept of Energy in Biosystems: Calorific value of food. Standard caloric content of carbohydrates, proteins and fats, Oxidation of food stuff (organic molecules) as a source of energy for cells. Introduction to Metabolism (catabolism, anabolism), ATP: the universal currency of cellular energy, ATP hydrolysis and free energy change. Conversion of food into energy. Outline of catabolic pathways of Carbohydrate- Glycolysis, Fermentation, Krebs cycle. Overview of catabolic pathways of Fats and Proteins. Interrelationships in the metabolic pathways of Proteins, Fats and Carbohydrates.

SUGGESTED TEXT BOOKS

1. G. Protein-Coupled Receptors: Structure, Signaling, and Physiology, Siehler S. and Milligan Cambridge University Press, 2010.
2. G-protein-coupled Receptors: Molecular Pharmacology, Vauquelin G. and Mentzer B. V Wiley, 2007.
3. GPCR Molecular Pharmacology and Drug Targeting: Shifting Paradigms and New Directions, Gilchrist A., Wiley, 2011.
4. Saenger, W. Principles of Nucleic Acid Structure Springer-Verlag (1984).
5. Sinden, R. P. DNA Structure and Function Academic Press (1994).

SUGGESTED REFERENCE BOOKS

1. Crowe J and Bradshaw T. (2010) Chemistry for the biosciences- The essential concepts. Oxford University Press, 2nd ed.
2. Principles of Biochemistry 6th edition, 2006 - Jeremy M. Berg, John L. Tymoczko and Lubert Stryer (W.H. Freeman & Co.)
3. Lehninger Principles of Biochemistry 5th edition, 2008 - Nelson, D. L. and M. M. Cox. (W. H. Freeman &Co.).
4. Outlines of Biochemistry 5th edition 2001- Conn, E.E., Stumpf, P. K. Bruening, G. and Doi, R.H. (JohnWiley and Sons).
5. Harper's Illustrated Biochemistry - R.K. Murray et al. (McGraw Hill)

Course Details			
Course Title: Green Chemistry I: Solvents & Synthesis			
Course Code	**MSCHE1003E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To make students understand the principles and goals of green chemistry
- To acquaint with the concept of green solvents and to understand the need for alternative solvents
- To develop an understanding of supercritical fluids, biphasic systems and ionic liquids
- To equip the students with necessary skills to do radiation-based synthesis

Learning Outcomes: After completion of the course the learners will be able to:

- Distinguish between a green-process and non-green process
- Design alternative routes of synthesis which is greener, cleaner and cost-effective
- Perform radiation based synthesis such as sonochemical and microwave
- Conduct solvent-less synthesis

UNIT-I

Introduction: Need for Green chemistry – Goals of green chemistry; principles of green chemistry with their explanations and examples – Designing a green synthesis – Prevention of waste / byproducts – Atom economy (maximum incorporation of materials used in the process) – Minimization of hazardous / toxic products – prevention of chemical accidents

UNIT-II

Green Solvents: Role of solvents in chemical synthesis, Environmental and health concerns of organic solvents, Need for Alternative/Cleaner solvents, Criteria for selection and design of green solvents
Water: the natural solvent on earth, organic reactions: hydrophobic effects enhancing the reaction selectivities, low solubility of O_2 in water, water soluble catalysts, challenges in using water as solvent,
Ionic liquids: physicochemical properties, Synthesis of Ionic Liquids, Directed Inorganic and Organometallic Synthesis, formation of oxides, electrochemical synthesis in ionic liquids,

Glycerol: solvent properties, volatility, polarity, availability, glycerol as a solvent combining the advantages of water and ionic liquids, enhancement of reaction selectivity, glycerol as a solvent for catalyst design and recycling, separation processes and material synthesis in glycerol, examples of synthesis of transition metal and metal oxide crystals

Supercritical fluids: supercritical CO_2 and its properties, advantages of using CO_2 as solvent, Synthesis of metal nanoparticles, CO_2 as solvent for coatings and lithography, biomaterial processing, other supercritical fluids.

Biphasic systems: Liquid-liquid interface, aqueous biphasic systems, phase- and micelle forming polymers for clean separation processes, Fluorous biphasic catalysis (FBC)

UNIT-III

Radiation based techniques in green synthesis
Microwave: microwave as a form of electromagnetic radiation, interaction of materials with microwaves and dielectric heating, microwave reactors, Different types of reactions involved in microwave synthesis (i) direct reactions, including those involving the use of simple compounds; Hoffann Elimination, Diels Alder reaction, (ii) preparation of solids which involve decompositions and combinations giving rise to solids of complex composition; (iii) nitridation reactions; (iv) reactions brought about in liquid media; (v) preparation of glasses; (vi) selective deoxidation reactions;and (vii) plasma-assisted reactions. Microwave synthesis of zeolite membranes & other examples
Sonochemical: ultrasound waves, basic principles of sonochemistry, acoustic cavitation phenomenon, Stable and transient cavitation, Temperatures of cavitation, Cold sono-fusion, Hydrodynamic cavitation, From cavitation to chemistry, generation of free radicals, sonochemical reactions, sono-oxidation, sono-reduction, sonication in ionic liquids, ultrasound and photochemistry, Combined use of ultrasound and microwaves, some examples of sonochemical synthesis. Esterification, Saponification

SUGGESTED TEXT BOOKS

1. Ionic Liquids in Synthesis, Peter Wasserscheid and Tom Welton, WILEY-VCH Verlag GmbH & Co. KGaA, 2008.
2. Green Chemistry and Catalysis, R.A. Sheldon, I. Arends and U. Hanefeld, WILEY-VCH Verlag GmbH & Co. KGaA (2007).
3. Green Solvents for Chemistry: Perspectives and Practice, William M. NelsonOxford University Press (2003).
4. Biocatalysis for Green Chemistry and Chemical Process Development, Junhua Tao and Romas Joseph Kazlauskas, WILEY-VCH Verlag GmbH & Co. KGaA (2011).
5. Green chemistry for chemical synthesis, Chao-Jun Li and Barry M. Trost, Proceedings of National Academy of Sciences (USA), year 2008, vol. 105, pages 13197–13202.
6. Advances in inorganic chemistry, Elsevier, Vol. 58, (2006).
7. Green Catalysis, Masaya Matsuoka and Masakazu Anpo, Wiley-VCH Verlag GmbH & Co. KGaA (2010).
8. A primer on electrocatalysis, J.O'M. BOCKRIS, J. Serb. Chem. Soc. 70 (3) 475–487 (2005).
9. Direct Electrochemistry of Hemoglobin and Its Electrocatalysis Based on Hyaluronic Acid and Room Temperature Ionic Liquid, Electroanalysis 20, 2008, No. 23, 2537 – 2542.
10. Photocatalysis. A multi-faceted concept for green chemistry, D.Ravelli, D. Dondi,M. Fagnonia and A. Albini, Chem. Soc. Rev., 2009, 38, 1999–2011.

11. Synthesis of Inorganic Solids Using Microwaves, K. J. Rao, B. Vaidhyanathan, M. Ganguli, and P. A. Ramakrishnan, Chemistry of Materials,. 1999, 11, 882-895.
12. Sonochemistry and sonoprocessing: the link, the trends and (probably) the future, Timothy J. Mason, Ultrasonics Sonochemistry 10 (2003) 175–179.

Course Details			
Course Title: Solid State and Structural Chemistry			
Course Code	**MSCHE2001E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To acquaint the students with the electronic and magnetic properties of the solids
- To introduce the emerging concepts of piezoelectricity, ferrolelectricity and dielectrics
- To equip the students with necessary skills in gometrical crystallography
- To make students learn the concepts and techniques of structure determination [x-ray diffraction (XRD), neutron diffraction (ND), electron diffraction (ED)]

Learning Outcomes: After completion of the course the learners will be able to:

- Identify the symmetry elements in a solid and assign a point group
- Explain the band structure of solids
- Understand and apply concepts of piezoelectricity, ferroelectricity in daily life
- Determine the crystal structure using XRD & ED

UNIT-I

Electronic structure of solids: Bonding in solids: Ionic, covalent, metallic and molecular solids free electron theory, Fermi sphere, Fermi-Dirac statistics, Ohm's law, limitations of the free electron theory.
Electrons in a weak periodic potential (Independent electron model), energy levels in extended, repeat and reduced zone schemes

Electrical and Magnetic Properties of Solids Metals: calculation of density of states, origin of resistivity, weak paramagnetism Semiconductors: Intrinsic and extrinsic- p and n-types, Hall effect, Junctions and their applications- metal-metal, metal-semiconductor, semiconductor-semiconductor types and transistors.
Insulators- dielectric properties, piezo and inverse piezoelectric effects, ferroelectricity, ferroelectric transitions in $BaTiO3$, ionic conductivity applications of band theory to TiO and NiO: Limitations of the Independent electron model, modelling electron correlation.

UNIT-II

Geometric Crystallography
Symmetry elements, Bravais lattices, Screw axes and glide planes, point groups, and space groups and nomenclature. Law of Interfacial angle (Euler's construction).
Diffraction theory and Single crystal X-ray diffraction

X-rays, Bragg's law, assignment of diffraction peaks, diffraction pattern of a primitive cubic lattice, space group extinctions, Scattering factor and structure factor, intensities from atomic positions for BCC and FCC lattices; Ewald's sphere of reflection, Reciprocal Lattice concept, Electron density function, Fourier synthesis, Fourier transform of the structure factor, Phase problem and Patterson synthesis.

UNIT-III

Experimental Methods: Rotation, Oscillation, Weissenberg and Precession methods. Debye-Scherrermethod (Powder method), Determination of lattice parameters from these methods.
Electron diffraction: Experimental technique, Wierl equation, Radial-Distribution method**.**

Neutron diffraction: Principle and Theory, advantages and uses.

SUGGESTED TEXT BOOKS

1. Introduction to Solids, L. V. Azaroff, McGraw Hill Book Co., New York, 1960.
2. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Holt Saunders International Ltd., New York (1976).
3. Physical Chemistry, G. M. Barrow, McGraw Hill (2nd ISE) (1966).
4. An Introduction to X-ray Crystallography, M. M. Woolfson, Cambridge University Press-Vikas Publishing House, New Delhi (1980).
5. Principles of the Solid State, H. V. Kheer, Wiley Eastern Ltd., New Delhi (1993).
6. Dynamics of Atoms in Crystals, W. Cochran, Edward Arnold, London, 1973. (Pages 24-37)
7. Vibrational Spectroscopy of Solids, P.M.A. Sherwood, University Press, Cambridge, 1972. (pages: 1-45)
8. Phase Transitions, C.N.R. Rao and K.J. Rao, Cambridge University Press
9. X-ray Structure determination: A practical guide, George H Stout and Lyle H Jenson, Macmillan Publishing Co.Inc and Collier Macmillan Publishers

SUGGESTED REFERENCE BOOKS

1. R. West, Solid State Chemistry and its Applications, John Wiley & Sons, 1984.
2. L. Smart and E. Moore, Solid State Chemistry - An Introduction, Chapman & Hall, 1992.
3. H. V. Keer, Principles of the Solid State, Wiley Eastern Limited, 1993.
4. K. Chakrabarty, Solid State Chemistry, New Age Publishers, 1996.

Course Details			
Course Title: Advanced Instrumental Techniques-I			
Course Code	**MSCHE2002E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To equip the students with the knowledge and skills in advanced instrumental techniques
- To develop a comprehensive understanding of diffraction based techniques such as X-ray Diffraction (XRD), Electron Diffraction (ED) and Neutron Diffraction (ND)
- To make students learn the core concepts of absorption spectroscopic techniques such as UV-Vis ansorption, FT-IR and Raman spectroscopy and its applications

- To impart knowledge and skills about the Resonance based techniques such as Mossbauer, NMR and EPR spectroscopy

Learning Outcomes

After completion of the course the learners will be able to:

- Deduce the lattice structure by analyzing the XRD, ED and ND patterns
- Analyze the UV-Vis absorption, vibrational (FTIR, Raman) and rotational (microwave) spectra
- Apply Mossbauer spectroscopy technique to explain the hyperfine properties of iron and tin compounds

UNIT I

Diffraction based techniques

X-ray diffraction: *Powder X-ray diffraction:* construction of the instrument, Identification of unknown materials, Determination of sample purity, Determination and refinement of lattice parameters, Determination of crystallite size/stress

Single-crystal X-ray diffraction: determination of crystal structure, position of H-atom in inorganic compounds, determination of bond lengths,

X-ray diffraction using synchrotron source: determination of complex molecules like proteins, enzymes. Neutron diffraction, electron diffraction

UNIT II

Absorption spectroscopy

UV-Vis absorption : construction of the instrument, measuring a spectrum, Beer-Lambert law, deviations from Beer's law, Relating UV-Vis spectra and colour, spectroscopic monitoring of titrations and kinetics

FT-IR and Raman spectroscopy: understanding the molecular vibrations and their energies, Complementary relationship between Raman and FTIR spectroscopy.

FTIR spectroscopy*:* construction of the instrument, dispersive and non-dispersive spectrometers, change dipole moments during molecular vibrations, Interferrogram and its Fourier Transformation, Far-IR, Mid-IR, Near IR spectral regions, optical windows: KBr, CsI pellet technique, Parraffin mulls, ZnSe, CaF_2 windows; Total internal reflectance based devices,

Raman Spectroscopy: Construction of the instrument, use of lasers as excitation source, Rayleigh scattering and Raman scattering, polarizability & molecular vibrations, Stokes lines and anti-Stokes lines, Resonance Raman technique, interpretation of a Raman spectra. Using FTIR and Raman spectra to determine geometry of a molecule, intermolecular interactions.

UNIT III

Resonance Techniques

Nuclear Magnetic Resonance (NMR):Construction of the instrument, basic principles, magnetic nuclei and Larmor precession, chemical shift and intensities of lines, spin orbit coupling, fluxionality, recording the spectrum, NMR of paramagnetic molecules, contact and dipolar shifts, ^{15}N, ^{19}F, ^{91}P NMR, NMR of heavy nuclei, Solid State- NMR

Electron Paramagnetic Resonance (EPR) or Electron Spin Resonance (ESR): Construction of the instrument, basic principles, the g-value, the hyperfine splitting, EPR of Transition metal ions: Spin Hamiltonian, spin-orbital coupling, g and A matrices, solutions to S=1/2 systems in various ligand fields, d^9, d^1, d^5 systems, S>1/2 systems, zero-field splitting – single crystal and powder spectra – spin-lattice and spin-spin relaxation, interpreting the superhyperfine coupling,

Mössbauer spectroscopy: the instrumental set-up, basic principles, emission of γ-radiation by radioactive ^{57}Co, resonant absorption of γ-radiation by nuclei, sensitivity of such absorption to the electronic and magnetic environment, interpreting the Mössbauer spectrum.

SUGGESTED TEXT BOOKS

1. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt, and J. A. Dean, 6th Edition (1986),
2. Quantitative Chemical Analysis, Daniel C. Harris

3. Spectrometric Identification of Organic Compounds, 7th Edition, Robert M. Silverstein, Francis X. Webster, David Kiemle.
4. William Kemp, Organic spectroscopy, Pal grave, New York.
5. Introduction to Spectroscopy. Donald L. PaviaGeorge, S. Kriz, James A. Vyvyan.
6. Fundamentals of Analytical Chemistry by A. Skoog and M. West
7. Vogel's Hand Book of Quantitative Analysis by Longman
8. Physical methods for chemists: R.S. Drago

SUGGESTED REFERENCE BOOKS

1. R. Wiesendanger, Scanning Probe Microscopy and Spectroscopy, Cambridge University Press, 1994.
2. Frank A. Settle, Handbook of instrumental techniques for analytical chemistry, Prince Hall, New Jersey, 1997.
3. K. W. Kolasinski, Surface science: Foundations of catalysis and nanoscience, John Wiley and Sons, West Susses, 2002.
4. D. A. Skoog, D. M. West, F. J. Holler and S. R. Couch, Fundamentals of analytical chemistry. Brooks/ColeCengage learning, New Delhi, 2004.
5. P. Atkins and J. de Paula, Atkins' physical chemistry, 8th Ed., Oxford University Press, New Delhi, 2008.
6. T. Pradeep, Nano: The essentials, McGraw-Hill Education, New Delhi, 2010.
7. F. Scholz, Electroanalytical Methods, Springer, 2nd Ed., 2010.

Course Details			
Course Title: Green Chemistry II: Catalysis			
Course Code	**MSCHE2003E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

To make students understand catalaysis as one of the fundamental pillars of green chemistry

- To acquaint the students with the fundamentals of electrocatalysis in biological systems and water-splitting reactions
- To develop a thorough understanding of photocatalysts and their different modes of action
- To familiarize with biocatalysis with respect to bioremediation of contaminats and to understand the enzyme-based methods of energy production

Learning Outcomes

After completion of the course the learners will be able to:

- Explain how biomimetic metal complexes are used as catalysts for various processes
- Design a catalyst to make a process greener
- Discuss the examples of naturally occurring photocatalytic reactions
- Underscore the importance of photocatalysts in exploiting the solar energy to drive difficult reactions
- Understand electrocatalysis with respect to water-purification and water-splitting reactions
- Discuss the bioremediation of contaminants and enzyme-catalyzed reacttions for gennerarting energy and biuels

UNIT I

Catalysts in Green Chemistry: Catalysis as one of the fundamental pillars of green chemistry, Catalyst design, Cu, Zn, Fe, Mn complexes as catalysts, Biomimetic Cu complexes for green oxidation of alcohols, catalysts that activate the natural oxidant hydrogen peroxide, TAML activators and its applications, aluminophosphate molecular sieve catalyst with cobalt(III) and Mn(III) ions, solid acid catalysts and the uses thereof, metal loaded silica as catalysts, Rh catalysts containing bisphosphanes and bisphosphites as chelating ligand, kaolinitic clay as catalyst.

UNIT II

Electrocatalysis: Electron Transfer Process, Multi-step Reactions, Electrolysis of water, Mechanism of hydrogen evolution, Choice of electrocatalysts for h.e.r, Electrocatalytic oxidation of NAD(P) H at mediator-modified electrodes, Electrocatalysis of Hemoglobin in ionic liquid, thin films and membranes, Electrocatalytic reduction of bromate ions for water purification.

UNIT III

Photocatalysis: Photocatalysis and green chemistry, photocatalytic processes in natureeg eg., photosynthesis, three basic ways of exploiting solar energy, photocatalysts and their modes of action, electron transfer, H abstraction, photocatalytic activity: the effect of surface area and electron-hole recombination,designa of photocatalysts of high activity Photocatalysis for producing hydrogen, TiO_2, other metal oxides, sulfides as photocatalysts, Photocatalysis in synthesis, photooxidation, photo-oxygenation, photoreduction, photocatalytic formation of C-C, C-N, C-X bonds, Photocatalytic remediation of environment, heterogeneous & homogeneous photocatalysis: the case of semiconductors and dyes

UNIT IV

Biocatalysis: Biocatalysis platform for green processes, Bioremediation of persistent contaminants, Microbial bioremediation, Enzymatic bioremediation, Laccases: blue enzymes for green chemistry, Laccases and chemical mediators: mimicking nature, laccases as biocatalysts for chemical reactions, optimum reaction condition for the enzyme, laccases in manufacturing industries, hyperthermophilic enzymes for biocatalysis, biophysical properties of the enzymatic breakers, Galactomannan as the supporting matrix for hydraulic fracturing of oil/gas wells, Enzymes for clean energy production, Amylolytic enzymes and bioethanol production, Biodiesel, biohydrogen and biofuel cells, High fructose corn syrup (HFCS) production, Thermophilic esterases, biocatalysis in ionic liquids, enzyme discovery

SUGGESTED TEXT BOOKS

1. Green Chemistry and Catalysis, R.A. Sheldon, I. Arends and U. Hanefeld, WILEY-VCH Verlag GmbH & Co. KGaA (2007).
2. Biocatalysis for Green Chemistry and Chemical Process Development, *Junhua Tao and Romas Joseph Kazlauskas*, WILEY-VCH Verlag GmbH & Co. KGaA (2011).
3. Green chemistry for chemical synthesis, *Chao-Jun Li and Barry M. Trost*, Proceedings of National Academy of Sciences (USA), year 2008, vol. 105, pages 13197–13202.
4. Advances in inorganic chemistry, Elsevier, Vol. 58, (2006).
5. Green Catalysis, *Masaya Matsuoka and Masakazu Anpo*, Wiley-VCH Verlag GmbH & Co. KGaA (2010).
6. A primer on electrocatalysis, J.O'M. BOCKRIS, J. Serb. Chem. Soc. 70 (3) 475–487 (2005)
7. Direct Electrochemistry of Hemoglobin and Its Electrocatalysis Based on Hyaluronic Acid and Room Temperature Ionic Liquid, Electroanalysis 20, 2008, No. 23, 2537 – 2542.
8. Photocatalysis. A multi-faceted concept for green chemistry, D.Ravelli, D. Dondi,M. Fagnonia and A. Albini, Chem. Soc. Rev., 2009, 38, 1999–2011.

9. Synthesis of Inorganic Solids Using Microwaves, *K. J. Rao, B. Vaidhyanathan, M. Ganguli, and P. A. Ramakrishnan,* Chemistry of Materials,. 1999, 11, 882-895
10. Sonochemistry and sonoprocessing: the link, the trends and (probably) the future, Timothy J. Mason, Ultrasonics Sonochemistry 10 (2003) 175–179.

Course Details			
Course Title: Nucleoside, Advances in Nucleic Acid and Proteins			
Course Code	**MSCHE2004E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

OBJECTIVE: To understand structures and functions of nucleic acid and proteins with a perspective of chemistry and biology and further integrate this for use in drug discovery and biotechnology.

Nucleoside: Modified nucleoside as a new drugs as antiviral and anticancer agents.

Nucleic acids: Definition, structure and properties, different type of base pairing, double helices, Sugar-Phosphate Chain conformations, conformation of DNA, physical properties and stability of DNA. DNA replication, genetic information storage, transcription, translation, transmission and gene expression, DNA intercalation, chemical synthesis of oligonucleotides, hybridization with synthetic oligonucleotides, characterization and purification techniques, nucleic acids as molecular probes. Catalytic RNA, siRNA, micro RNA. DNA damages, mutations and repair. Modified nucleic acids: Peptide nucleic acids (PNAs), LNAs, synthesis of PNAs, doubly labeled PNAs as probes for the detection of point mutations. Single Nucleotide Polymorphism (SNPs).

Proteins: Different strategies and methods for the production, isolation, structure determination, functional analysis and modification of proteins, analyse and interpret protein sequences and structures and use such information to predict protein function, Understanding of fundamental concepts of proteomics and hands-on experience with techniques used in current proteomics. Use of protein for production and development of drugs, for biotechnological and other industrial and scientific purposes and explaination how this is facilitated by knowledge of the structure and function of proteins.

SUGGESTED BOOKS

1. C.M. Dobson, J.A. Gerrard and A.J. Pratt., Foundations of Chemical biology, Oxford University Press 2002.
2. A. Miller and J. Tanner, Essentials of Chemical Biology, Willey & Sons Ltd. 2008. References: 1. S. L. Schreiber, T. Kapoor and G. Wess, Chemical Biology: from small molecules to systems biology and drug design, Wiley – VCH Verlag GmbH & Co. 2007.
3. S. L. Schreiber, T. Kapoor and G. Wess, Chemical Biology: from small molecules to systems biology and drug design, Wiley – VCH Verlag GmbH & Co. 2007.
4. Stryer, L.; Berg, J. M.; Tymoczko, J. L. In Biochemistry, 5th Ed. (Hardcover).
5. Lehninger Principles of Biochemistry, 5th Ed. by Nelson and Cox.
6. McLaughlin, L. W.; Wilson, M.; Ha, S. B. Use of Nucleoside Analogues to probe Biochemical Processes
7. (a) Wojciechowski, F.; Leumann, C. J. Chem. Soc. Rev. 2011, 40, 5669. (b) Jan Stambasky, Michal Hocek and Pavel Kotovsky Chem. Rev., 2009, 109, 6729.

8. (a) Kool, E. T.; Morales, J. C.; Guckian, K. M. Angew. Chem. Int. Ed. 2000, 39, 990. (b) Kool, E. T. Acc. Chem. Res. 2002, 35, 936. (c) Teo, Y. N.; Wilson, J. N.; Kool, E. T. J. Am. Chem. Soc. 2009, 131, 3923. (d) Schweitzer, B. A.; Kool, E. T. J. Am. Chem. Soc. 1995, 117, 1863. (e) Kool, E. T. Annu. Rev. Biochem. 2002, 71, 191. (f) Jarchow-Choy, S. K.; Sjuvarsson, E.; Sintim, H. O.; Eriksson, S.; Kool, E. T. J. Am. Chem. Soc. 2009, 131, 5488.

Course Details			
Course Title: Chemistry of Natural Products			
Course Code	**MSCHE2005E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

OBJECTIVE: To give students an awareness of the richness and diversity of plants and animal around us. To make students aware of the many pharmaceutically active products of natural origin. To learn the origin of natural products, their characterisation and synthesis.

Course Outcome: At the end of the course, students should be able to: The knowledge of the students is enhanced with the clear information about the natural products which are having medicinal importance.

- Identify and characterize various classes of natural products by their structures;
- Appreciate the biogenesis of many natural products of importance.

UNIT-I

Basics of Metabolism (primary & secondary), Reactive Intermediates in Biosynthesis, Role of ATP and other important important coenzyme, catabolism, anabolism, biosynthesis of terpenoids alkaloids, and other natural products.

UNIT-II

Terpenoids and Carotenoids: Classification, nomenclature, occurrence and isolation. Isoprene rules. Stereochemistry of citral, farnesol, limonene, 1, 8-cineole, menthols and borneols. Correlation of configurations of terpenoids.

Structure elucidation of camphene, pinene, caryophyllene, santonin and gibberrillic acid. Synthesis and biosynthesis of the following: Linalool, -terpineol, Commercial synthesis of camphor.

UNIT-III

Alkaloids: Definition, nomenclature, occurrence, isolation, classification, General methods of structure elucidation. Synthesis and biosynthesis of the following alkaloids: Ephedrine, hygrine, coniine and cocaine.

UNIT-IV

Steroids: Occurrence. Nomenclature, basic skeleton, Diels hydrocarbon and stereochemistry. Isolation, structure and structural elucidation of sterols and bile acids. Cholesterol.

UNIT-V

Porphyrins and vitamin B_{12}: Structure elucidation and synthesis of haemin, chlorophyll-a and vitamin-B_{12}

Prostaglandins: Introduction, nomenclature, classification and biological role of prostaglandins. Synthesis of PGE_1 and PGE_2 by Corey's and Stork's approaches.

Insect pheromones: Introduction, classification. Pheromones in pest control. Syntheses of (one synthesis should be stereoselective synthesis)

SUGGESTED BOOKS

1. Natural products: Their chemistry and biological significance-J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthorpe & J. B. Harborne, Longman, UK, 1994.
2. Terpenes, J. Verghese, Tata McGraw-Hill, New Delhi, 1982.
3. Chemistry of terpenes and terpenoids, A. Newman, Academic Press, London, 1975.
4. Handbook of naturally occurring compounds Vol. II: Terpenes, T. K. Davon, A. I. Scott, Academic Press, NY, 1972.
5. Natural products chemistry Vol. I & II, K. Nakanishi, T. Goso, S. Ito, S. Natori & S. Nozoe, Academic Press, NY, 1974.
6. Total synthesis of natural products Vol. I & VI, Apsimon, John Wiley, NY, 1973-1981.
7. Organic chemistry Vol.II, I. L. Finar, 6th Edn. Longman, 1992.
8. Chemistry of natural products Vol. I & II, O. P. Aggarwal, Goel Publishing House, 6th Edn. 1982.
9. Total synthesis of natural products: The chiral approach Vol.III, S. Hanessian Pergamon Press, 1983.
10. Total synthesis of steroids, Akhaun & Titov, Jerusalem, 1969.
11. Medicinal natural products: A biosynthetic approach, P. M. Dewick. John Wiley, Chichester, 1997.
12. Chemistry of natural products: A unified approach, N. R. Krishnaswamy, University Press, India, 1999.
13. Medicinal natural products: A biosynthetic approach, P. M. Dewick. John Wiley, Chichester, 1997.

Course Details			
Course Title: Atom Dynamics in Solid and Advanced Magnetochemistry			
Course Code	**MSCHE3001E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To enhance the understanding of the electronic structure of solids
- To acquaint the students with the advanced level concepts in magnetochemistry such as magnetic anisotropy and single molecule magnets
- To familiarize the students with the concepts of piezoelectricity, ferrolelectricity, dielectrics and superconductivity
- To impart the knowledge and skills in electrochemical aspects of inorganic systems

Learning Outcomes: After completion of the course the learners will be able to:

- Distinguish between piezoelectric and ferroelectric effects in inorganic systems
- Understand and apply concepts of piezoelectricity, ferroelectricity in daily life
- Determine the magnetic anisotropy and susceptibility in inorganic systems
- Apply the advanced concepts in designing single molecule magnets
- Apply the concepts of defects-engineering to obtain enhanced features of inorganic systems
- Explain the electrochemical proceses occurring in biological systems
- Apply the concepts for protection from corrosion

UNIT-I

Electronic structure of solids: Bonding in solids: Ionic, covalent, metallic and molecular solids.
Free electron theory, Fermi sphere, Fermi-Dirac statistics, Ohm's law, limitations of the free electron theory Electrons in a weak periodic potential (Independent electron model), energy levels in extended, repeat and reduced zone schemes
Electrical and Magnetic Properties of Solids: Metals: calculation of density of states, origin of resistivity, weak paramagnetism Semiconductors: Intrinsic and extrinsic- p and n-types, Hall effect, Junctions and their applications- metal-metal, metal-semiconductor, semiconductor-semiconductor types and transistors.
Insulators- dielectric properties, piezo and inverse piezoelectric effects, ferroelectricity, ferroelectric transitions in BaTiO3, ionic conductivity applications of band theory to TiO and NiO: Limitations of the Independent electron model, modeling electron correlation.

UNIT II

Advanced Magnetochemistry: Definition of magnetic properties, types of magnetic bodies, Curie equation, Curie's law and Curie-Weiss law. Anisotropy in magnetic susceptibility, diamagnetism in atoms and polyatomic system, Pascal's constants, two sources of paramagnetism, spin and orbital effects, spin-orbit coupling, Lande interval rule, energies of J levels, first order and second order Zeeman effects, temperature independent paramagnetism, simplification and application of van Vleck susceptibility equation, quenching of orbital moment, magnetic properties of transition metal complexes, low spin, high-spin crossover, magnetic behavior of lanthanides and actinides, magnetic exchange interactions. Molecular magnets, Single Molecule Magnets (SMMs), 3d, 4f and 3d-4f based SMMs. Experimental arrangements for determination of magnetic susceptibility: SQUID.

UNIT-III

Dynamics of Atoms in a Solid: Dispersion curves of an elastic structureless medium, Longitudinal and Transverse modes, Optical and Acoustic modes of a crystal, total vibrational energy of a crystal. Case study of calcite.
Defects in Solids: Point defects, Line defects and Plane defects, Stacking faults and grain boundaries.
Superconductivity: Superconductivity, Meisner effect, Type I and type II superconductors, Features of superconductors, Frolich diagram, Cooper pairs, Theory of low temperature superconductivity, Junctions using superconductors.
Phase Transition in Solids: Definitions, Classification of phase transitions, First and second order phase transitions: Martensitic transition, order-disorder transitions and spinodal decomposition.

UNIT IV

Electrochemical aspects of inorganic systems: Electrochemical synthesis: Special features of electrochemical synthesis compared to conventional synthesis-reaction variables (electrode material, electrode potential, solvent, supporting electrolyte, temperature, agitation) in electrochemical synthesis. Examples of electro-inorganic and electrochemical nanoparticles synthesis with mechanism.
The electrochemical interface between biomolecules, cellular membrane, transmembrane potential, bilayer lipid membranes, electroporation, biological electron transport, electrochemistry of redox enzymes, biological membrane and membrane mimics. Biosensors- NADP, glucose, phenolic. Bioelectroanalysis: Electrolysis and Electrodialysis.
Corrosion and its prevention: Cathodic protection, anodic protection, use of corrosion inhibitors, use of organic coatings

SUGGESTED TEXT BOOKS

1. Inorganic Electrochemistry: Theory, Practice and Application, Piero Zanello, Royal Society of Chemistry, London, 2007
2. Molecular Electrochemistry of Inorganic, Bioinorganic and Organometallic Compounds *Volume 385 of Nato Science Series C:*, A.J.L. Pombeiro, J.A. McCleverty, Springer Science & Business Media, 2012
3. Introduction to Magnetochemistry, Alan Earnshaw, Elsevier, 2013
4. Physical principles and applications of magnetochemistry, Sir Shanti Swarupa Bhatnagar, K. N. Mathur, Macmillan and Co., limited, 1935
5. Magnetochemistry, Richard L. Carlin, Springer Science & Business Media, 2012
6. Solid State Chemistry and its Applications, Anthony R. West, 2nd Edition, John Wiley & Sons, 2014

SUGGESTED REFERENCE BOOKS

1. Dynamics of Atoms in Crystals, W. Cochran, Edward Arnold, London, 1973. (Pages 24-37)
2. Vibrational Spectroscopy of Solids, P.M.A. Sherwood, University Press, Cambridge, 1972. (Pages: 1-45)
3. Phase Transitions, C.N.R. Rao and K.J. Rao, Cambridge University Press
4. X-ray Structure determination: A practical guide, George H Stout and Lyle H Jenson, Macmillan Publishing Co.Inc and Collier Macmillan Publishers.
5. Solid State Chemistry: An Introduction, Fourth Edition, Lesley E. Smart, Elaine A. Moore, CRC Press, 2016
6. Electrochemistry of Metal Complexes: Applications from Electroplating to Oxide Layer Formation, Arvydas Survila, John Wiley & Sons, 2015
7. Biological Electrochemistry, Volume 1, Glenn Dryhurst, Elsevier, 2012

Course Details			
Course Title: Surface Phenomena, Chemical Dynamics and Spectroscopy			
Course Code	**MSCHE3002E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To develop comprehensive understanding of chemical kinetics snad catalysis
- To make students understand the catalysis occurring in biological systems
- To impart knowledge of surface structure and skills in analysing the adsorption phenomena through different typs of isotherms, eg, Gibbs, BET , Langmuir etc
- To make the students understand colloids and related phenomena and correlate it with examples in daily life
- To equip the students with necessary knowledge and skills in spectroscopy, namely, rotational, vibrational and electronic spectroscopy

Learning Outcomes: After completion of the course the learners will be able to:

- Explain the catalysis by enzymes in biosystems
- Determine the rate constant and design a catalyst
- Determine the binding affinity of anlyte on a surface using Langmuir or BET isotherms
- Design collodal systems with enhanced stability and use it for solving problems in daily life
- Analyse spectroscopic data for identification of compound and use it for understanding intemoloecular interactions.

UNIT I

Chemical Dynamics –II: Kinetics of homogeneous catalysis-kinetics of auto catalytic reactions, kinetics of acid-base catalysed reactions. Comparison of enzyme catalysed and chemical catalysed reactions, Mechanism (Lock and Key theory), Kinetics of enzyme catalyzed reactions – Henri-Michaelis- Menten mechanism, Significance of Michaelis-Menten constant, Lineweaver-Burk plot. Effects of enzyme concentration, pH, Temperature, Activators and Inhibitors on enzyme activity. Theories of unimoleuclar reactions.

UNIT II

Surface and Colloids: Types of adsorption isotherms, Effect of temperature on adsorption, Mechanical adsorption, Estimation of surface area using BET equation, Gibbs adsorption isotherm and its significance, Surface tension and surface energy, Pressure difference across curved surface (Laplace equation), Vapour pressure of droplets (Kelvin equation), Surface film on liquids (electro-kinetic phenomena), Catalytic activity of surfaces.

UNIT-III

Rotational Spectroscopy: Rotations of molecules, rigid diatomic molecule- rotational energy expression, energy level diagram, rotational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, effect of isotopic substitution, centrifugal distortion and the spectrum of a non-rigid rotor.

Rotational spectra of polyatomic molecules- linear, symmetric top and asymmetric top molecules.

UNIT-IV

Infrared Spectroscopy-I: Vibrations of molecules, harmonic and anharmonic oscillators- vibrational energy expression, energy level diagram, vibrational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, hot bands, effect of isotopic substitution.

Diatomic vibrating rotor, Born-Oppenheimer approximation, vibrational-rotational spectra of diatomic molecules, P, Q and R branches, breakdown of the Born-Oppenheimer approximation.

Infrared Spectroscopy-II: Vibrations of polyatomic molecules: Normal coordinates translations, vibrations and rotations, vibrational energy levels and wave functions, fundamentals, overtones and combinations.

Vibration-rotation spectra of polyatomic molecules- parallel and perpendicular vibrations of linear and symmetric top molecules Techniques and instrumentation.

UNIT-V

Electronic Spectroscopy: Born-Oppenheimer approximation, vibrational coarse structure, intensities by Franck- Condon principle, Dissociation energy, rotational fine structure, Fortrat diagram, pre-dissociation, Electronic structure of diatomic molecules- basic results of MO theory, classification of states by electronic angular momentum- and molecular orbitals, selection rules, spectrum of singlet and triplet molecular hydrogen**,** Electronic spectra of polyatomic molecules- localized MOs, spectrum of HCHO, change of shape on excitation**,** Decay of excited states- radiative (fluorescence and phosphorescence) and non-radiative decay, internal conversion.

SUGGESTED BOOKS

1. Introduction to Molecular Spectroscopy, C. N. Banwell, TMH Edition (1994).
2. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill (Int. Students Edition) (1988).
3. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill (Int. Students Edition) (1990).
4. Spectroscopy, Vols. 1-3, B. P. Straughan and W. Walker, Chapman Hall (1976).

Course Details			
Course Title: Chemistry of Materials			
Course Code	**MSCHE3003E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To impart knowledge about the advanced materials and its characteristics
- To equip the students with skills in materials synthesis
- To make students aware of new emerging materials such as fullerrides, perovskites, NASCION and conducting polymers
- To acquaint the students with the salient features of nanomaterials
- To make students learn about the structure and properties of intercalation compounds, composites and amorphous materials

Learning Outcomes

After completion of the course the learners will be able to:

- Explain the relevance of advanced materials in daily life
- Distingush between different type of materials based on structure and properties.
- Synthesize materials using different methods such as sol-gel, spray pyrolysis, combustion, hydrothermal, electrosynthesis etc.
- Analyze properties of different types of materials such as nanomaterials, intercalation compounds, perovskites etc.

UNIT-I

Preparative Techniques: Principles of solid state synthesis- ceramic methods, solid solution and compound precursors (nitrates, carbonates, hydroxides, cyanides and organometallics), sol-gel, spray pyrolysis, combustion, hydrothermal, electrosynthesis

New Materials: Fullerenes and fullerides– structure, synthesis, functionalization approaches, conducting properties of fullerides and applications.

NASICON and alumina – structure and conducting properties.

High-T_C Oxides - structure, perovskite A & B, structure and synthesis of La, Sr and Ba cuprates, applications.

Conducting polymers - PA, PPP, PPS, PPY-mechanism of conduction and applications.

UNIT-II

Nanomaterials: Classification, types of carbon nano tubes, synthesis, functionalization charecterization and applications.

Principles of self-assembly: surfactant solutions, importance of non-covalent forces, the hydrophobic effect, co-operativity, statistical mechanics of one-dimensional self-assembly. Preparation of nanoscale materials: Precipitation, mechanical milling, colloidal routes, self-assembly: chemical vapour depostition, sputtering, evaporation.

Synthesis, characterization and applications of nanoparticles, nano wires and nanotubes. Elemental nanoparticles: Pure, Gold, Silicon, Silver, c o b a l t , Oxide nanoparticles: Silica, Zinc oxide, Iron oxide, Alumina.

UNIT-III

Intercalation Compounds: Intercalation reactions **-** layered structure-graphite interlayer compounds (GILC), staging of graphite, TaS_2, Microporous materials – zeolites and zeolitic materials, $AlPO_4$- $GaPO_4$.

Fibres and Composites: Synthetic inorganic polymers- zirconia and other fibre Classification, microscopic composites, dispersion strengthned, particle reinforced, Fibre-glass reinforced composites, metal-matrix, plastic-matrix composites, hybrid composites.

Amorphous Materials: Crystalline versus amorphous solids, glass formation, Prepararion techniques-meltspinning, sputtering, ion implantation, Structural models of amorphous materials, Properties of metglasses - mechanical, electronic and magnetic properties.

SUGGESTED BOOKS

1. Encyclopedia of Nanomaterials and Nanotechnology Hari Singh Nalva
2. Nanostructured Materials: Processing, Properites and Applications, ed. C.C.Koch, Willaim Andrew Publishing, New York, 2002.
3. Nanomaterials: Synthesis, properties and applications, Ed. By A.S.Edelstein and R.C. Cammarata, Inst. of Physics, UK 1966.
4. Science of Engineering Materials, C.M. Srivastava and C. Srinivasan, Wiley-Eastern Ltd. (1991).
5. Solid State Chemistry and its Applications, A.R. West, John Wiley & Sons.(1989).
6. Material Science and Engineering. W.D. Callister, John Wiley and Sons Inc. (1985).
7. Nanotubes and Nano wires CNR Rao, & A Govindaraj, RSC, London 2005.
8. NANO: The essentials T. Pradeep, McGraw-Hill, 2008.
9. Liquid Crystals, Nature's delicate phase of matter, Peter J Collings, Princeton University Press, 2002.
10. Nanochemistry, A chemical approach to Nanomaterials, Geoffrey A Ozin and Andre C Arsenault, RSC, 2006.

Course Details			
Course Title: Advanced Photochemistry			
Course Code	**SCHE3004E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To further renhance the understanding of photochemistry
- To make students learn the physicochemical properties of electronically excited state
- To acquaint students with the environmental eefects on absorption and emission spectra
- To develop an understanding of different types of photochemical reactions
- To impart knowledge about emerging topics such as photoeletrochemistry, photovoltaics and photosplitting of water

Learning Outcomes: After completion of the course the learners will be able to:

- Draw Electronic, vibrational, rotational energies-potential energies diagram and explain the photochemical processes
- Distinguish between photoluminescence, electroluminescence and chemiluminesce
- Discuss the effect of solvents on absorption and emission spectra
- Analyze a photochemical reactiom, determine the rate constant and photochemical quantum yield
- Discuss the role of photochemical processes in photovoltaics and generation of hydrogen energy

UNIT I

Importance of Photochemistry, Laws of Photochemistry: Grothus –Draper Law, Stark-Einsteins Law, Laws of light absorption, Quantum yield and numerical problems. Photochemistry and spectroscopy, units and dimensions. Electronic energy states of atoms, term symbols for atoms, energy levels for the electronic configuration of carbon and oxygen illustrating spin orbit coupling and Hunds rules, inverted multiplets as applied to simple atoms and also for inner transition metals, Laporte's selection rules. Physicochemical Properties of electronically excited molecules: Nature of changes on electronic excitation: acidity, dipole moment, redox potentials etc. Fates of excited species, Electronic, vibrational, rotational energies-potential energies diagram. Shapes of absorption band and Franck Condon principle.

UNIT II

Quantum mechanical formulation of Franck Condon, crossing of potential energy surfaces, Non crossing rule of Teller for potential energy surface. Emission spectra, fluorescence and phosphorescence

Environmental effect on absorption and emission spectra, solvent red shift and blue shift in absorption spectra. Experimental techniques to determine the intermediates in photochemical reactions
Classification of photochemical reactions, Rate constants and life times of reactive energy state Effect of light intensity on the rate of photochemical reaction Photo-fragmentation of photodissociation-Gas phase photolysis.

UNIT III

Photosensitized reaction, photofragmentation in liquid phase, photodegradation of polymers, Isomerization and other rearrangement reactions, Atmospheric photochemistry

Some current topics in photochemistry:

Semiconductors: Bonding and conductivity, mechanism of conductivity, energy bands in semiconductors, impurity semiconductors.
Photo voltaic effect: p-n junction solar cells, silicon cells, GaAs solar cells, schottky barrier solar cells.
Photoelectrochemistry: Introduction, efficiency of conversion of light to chemical and electrical energy, frequently measured quantities. Photosplitting of water using colloidal suspensions Photocatalysis: Photocleavage of waste which are environmentally hazardous by using TiO2, Photooxidation and photoreduction reactions.

SUGGESTED BOOKS

1. Fundamentals of photochemistry, K.K. Rohatgi Mukhergee, Wiley Eastern Limited (1986)
2. Photochemistry, Carol E Wayne and Richard P Wayne, Oxford University Press (1996)
3. Introduction to Semiconductor Materials and devices M S Tyagi, John Wiley and sons (1991)
4. Organic Photochemistry, J. M. Cozen and B. Halton, Cambridge University Press (I st Edition) 1974
5. Molecular Reactions and Photochemistry, C H Deputy and D S Chapman, Prentice Hall India, New Delh (1st Edition), 1972.

SUGGESTED REFERENCE BOOKS

1. Principles of Fluorescence Spectroscopy, 3rd Ed., J. R. Lakowicz, Springer, New York, 2006.
2. Fundamentals of Photoinduced Electron Transfer, G. J. Kavarnos, VCH publishers Inc., New York, 1993.
3. Molecular Fluorescence: Principles and Applications, B. Valeur, Wiley-VCH Verlag GmbH, Weinheim, 2002.
4. Modern Molecular Photochemistry of Organic Molecules, N. J. Turro, V. Ramamurthy, J. C. Scaiano, University Science, Books, CA, 2010.
5. Photochemical Synthesis, I. Ninomiya, T. Naito, Academic Press, New York, 1989.

Course Details			
Course Title: Medicine and Agrochemicals			
Course Code	**MSCHE3005E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

OBJECTIVE: Be familiar with several interdisciplinary areas of biochemistry, medicinal and pharmaceutical Chemistry and understanding the concepts in relation to application towards drug developments. To provide an appreciation of the importance of modern agrochemicals and the factors involved in their discovery.

UNIT I

Medicine from Nature: Introduction, the search for new medicine, secondary metabolite, elucidation of biosynthetic pathways for terpenoids, alkaloids and few well known compounds like erythromycin, rampamycin etc. genetic engineering of natural product biosynthesis.

UNIT II

New Medicine: Historical development of medicine, Drugs targets, Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (Aspirin, paracetamol, lbuprofen); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam),Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone).

Selected Examples of Drug Action at some Common Target Areas:

- Anesthetics: Classification, Characteristic features, Mechanism of action of general anesthetics
- Analgesics: antipyretic analgesics, opiate analgesics, non-steroidal Anti-inflammatory Drugs, mechanism of action
- Antihistamines: mechanism of action
- Antibiotics: Sulpha drugs, mechanism of action, β-Lactam antibiotics: Penicillinsepam), Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone).

UNIT III

Pesticides: Introduction, Insecticides, herbicides, fungicides.
Insecticides: Disrupters of the nervous system, insect growth regulators, respiration inhibitors, photosynthesis disrupters, hormone mimics, inhibitors of amino acid synthesis, inhibitors of lipid synthesis
Fungicides: Membrane disrupters, inhibitors of energy production, inhibitors of cell division, inhibitors of sterol synthesis.

SUGGESTED TEXT BOOKS

1. Surprise! A fungas factory for taxol? Science, 260, 154, 1993.
2. Introduction to alkaloids, G.A.Cordell, Wiley, 1981.
3. Secondary metabolism, J. Mann, Clarendon Press, Oxford, 1978.
4. Chemistry and mode of action of cope protection agents, I. G. Copping, RSC, 1998.
5. Insecticides with novel modes of action, I. Ishya and D. Degheele springer, 1998.
6. Pesticides Chemistry, G. Motolcsy, M. Nadasy and V. Andriska, Elsevier.

7. Fundamentals of Medicinal Chemistry, Gareth Thomas, John Wiley & Sons Inc
8. The Organic Chemistry of Drug Design and Drug Action, Richard Silverman, Mark W Holladay Academic Press, 2014.
9. Introduction to medicinal chemistry: How drug work, Grinauz Alex,Wiley VCH
10. Principles of Organic Medicinal Chemistry, R. R. Nadendla, New Age International, New Delhi, 2005.
11. Modern Drug Synthesis by Jie Jack Li and Douglas S. Johnson, (Wiley Series on Drug Synthesis)
12. Strategies for Organic Drug Synthesis and Design by Daniel Lednicer, Wiley
Burger's Medicinal Chemistry, Drug Discovery and Development, 7th Edition, Volume 3

Course Details			
Course Title: Nano Chemistry			
Course Code	**MSCHE3006E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

To acquaint the students with the fundamentals of nanoscience and nanotechnology

- To make students learn the structure and properties of different types of nanomaterials such as luminescent, superparamagnetic and plasmonic nanocrystals etc.
- To equip the students with necessary knowledge and skills in synthesis and characterization of nanomaterials
- To develop an understanding of self-aseembly and nanocatalysis
- To create awareness about applications of nanotechnology for energy generation, water purification, sensing, and healthcare

Learning Outcomes

After completion of the course the learners will be able to:
- Explain the nanomaterials as low dimensional systems and explain their properties
- Discuss and describe the salient features of nanomaterials such as quantum dots, plasmonic nanoparticles, superparamgnetic particles, CNTs and graphene
- Synthesize nanomaterials and characterize it using various techniques.
- Exaplin how the nanoparticles can be used as building blocks to create hierarchial nano/microstructures
- Discuss the origin of enhanced catalytic efficiency of nanoparticles
- Underscore the importance of nanotechnology in daily life through applications in solar cells, water purification anddiagnosis and therapy

UNIT-I

Introduction to Nanoscience & Nanotechnology: Introduction to the nano- the length scale, meaning of the terms nanomaterials, nanoscience and nanotechnology, nanotechnology currently in use, Histotical perspectives, Nature’s perspectives

Nanomaterials as low dimensional systems, classification into 2D, 1D and 0D systems. Electronic structure of such systems; Stabilization of colloidal nanoparticles, electrostatic and steric stabilization, surface functionalization of nanoparticles. Classification of nanomaterials based on their properties: Semiconductor nanoparticles: Quantum confinement effects, Quantum dots, quantum wells, quantum wires; size dependent absorption and emission of light (luminescence); Magnetic nanoparticles: superparamagnetism, SPIONs, Giant magnetoresistance (GMR) Plasmonic nanoparticles: surface plasmon resonance, Carbon based nanomaterials:

carbon nanotubes, fullerenes, graphenes, carbon dots, electron emission from CNTs, conductivity and enhanced catalytic activity compared to the same materials in the macroscopic state.

UNIT-II

Synthesis and Characterization of Nanomaterials: Top-down, bottom-up approach, liquid-phase synthesis, gas-phase synthesis, vapour-phase synthesis; Stabilization of nanoparticles, Surface passivation & functionalization, bioconjugation, direct absorption, covalent coupling.

Chemical Methods:- Arrested precipitation, coprecipitation; Metal nanocrystals by reduction, Sol-gel synthesis; Microemulsions or reverse micelles, solvothermal synthesis; Thermolysis routes, Microwave synthesis; Sonochemical synthesis; electrochemical synthesis; photochemical synthesis, Synthesis in supercritical fluids.

Physical Methods**:** Inert gas condensation, Arc discharge, Plasma arc technique, RF plasma, Ion sputtering, Laser ablation, Laser pyrolysis, Ball Milling, Molecular beam epitaxy, Chemical vapour deposition method, Physical vapor deposition, nanolithography and nanoindentation

characterization: Structural Characterization; size shape and crystal structure, Transmission electron microscopy(TEM),Scanning electron microscopy (SEM), Electron diffraction (ED), X-ray –diffraction (XRD), Atomic force microscopy (AFM), Dynamic light scattering (DLS) , Small angle X-Ray Scattering (SAXS),Neutron Scattering, Magnetic Characterization**:** determination magnetic susceptibility, coercivity etc, by SQUID, Vibrating sample magnetometer (VSM), Optical Characterization: UV-Vis absorption spectroscopy, Luminescence Spectroscopy.

UNIT-III

Self-Assembly of nanomaterials and Nanocatalysis: Nanoparticles as building blocks, Process of self-assembly, semiconductors islands, Self-assembled Monolayers (SAMs); crystal dipole directed self-assembly of nanoparticles into one dimensional and two dimensional nanostructures, self-assembly into three dimensional superlattices, such examples of semiconductor quantum dots; Self-assembly directed by molecular recognition, protein-directed self-assembly, dendrimer directed self-assembly, nucleic acid directed self-assembly, examples of metal/metal oxides/semiconductor nanoparticles.

UNIT-IV

Applications of Nanotechnology: Sensing Applications: Electrochemical sensors, Chemical sensor, physical sensors, biosensors, Nanostructured Gas Sensors, Colorimetric and fluorescent sensors for trace Contaminants in water, Detection of pesticides and explosives

Biomedical Applications: Luminescent NPs for imaging of cancer cells, Superparamagnetic Magnetic NPs for MRI (Magnetic resonance imaging), Noble metal NPs for imaging applications, Targeted Drug Delivery Meosporous silica/ Polymeric nanoshells/nanopartices for drug delivery; Liposomes and micelles as nanocarriers metal/semiconductor/polymeric nanoparticles Photodynamic therapy (PDT), Photothermal therapy (PTT) by plasmonic nanomaterials, Hyperthermia treatment by magnetic NPs.

Energy Applications: Solar energy for electricity production: photovoltaic nanotechnology, artificial photosynthesis Nanotechnology for: Hydrogen production, Hydrogen transport and storage, Hydrogen conversion, fuel.

SUGGESTED TEXT BOOKS

1. A Textbook of Nanoscience and Nanotechnology, T. Pradeep, Tata McGraw Hill Education Private Limited, New Delhi (2012).
2. Nanochemistry: A Chemical Approach to Nanomaterials, Geoffrey A. Ozin, André C. Arsenault, Ludovico Cademartiri, Royal Society of Chemistry (2009).

3. Concepts of Nanochemistry, Ludovico Cademartiri, Geoffrey A. Ozin, Jean-Marie Lehn, WILEY-VCH Verlag GmbH & Co. KGaA, (2009).
4. Nano: the Essentials, T. Pradeep, Tata McGraw Hill Education Private Limited, New Delhi (2007)
5. Environmental Applications of Nanomaterials, Glen Fryxell and Guozhong Cao, Imperial College Press, London (2007).
6. Introduction to nanotechnology, C. P. Poole Jr, F. J. Owens, 2nd edition, Wiley-India, Delhi, 2008.
7. Nanostructures and nanomaterials, G. Cao, Imperial College Press, University of Washington, USA, 2004.
8. Nanotechnology Fundamentals and applications, M. Karkare, I. K. international publishing house pvt. Ltd., Bangalore, 2008.
9. Springer Handbook of Nanotechnology, B. Bhusan, 3rd edition, Springer-Verlag, 2009.
10. Chemistry of Nanomaterials: Synthesis, Properties and Applications, CNR Rao and T. Cheetham, Wiley & Sons, 2005.
11. Nanoparticles: From Theory to Application, Günter Schmid, WILEY-VCH Verlag GmbH &Co. KGaA, (2011).
12. Nanoparticles: synthesis, stabilization, passivation, and functionalization, Ramanathan Nagarajan, T. Allan Hatton, Publisher: American Chemical Society (2008).
13. Magnetic nanoparticles, S. P. Gubin, WILEY-VCH Verlag GmbH & Co. KGaA,(2009)
14. Multifunctional Nanoparticles for Drug Delivery Applications: Imaging, Targeting, andDelivery, Sonke Svenson, Robert K. Prud'Homme, Springer (2012).

Course Details			
Course Title: Reaction mechanism, Organometallics and Advanced Bioinorganic Chemistry			
Course Code	**MSCHE4001E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To develop comprehensive understanding of reaction mechanism involving metal complexes
- To make students understand the role of organometallics in industrial catalysis and medicine
- To impart knowledge of structure and functions of metalloproteins
- To make the students understand the mechanism of metal ion transport across the cell membrane and discuss the toxicity of metals
- To impress upon the sudents the versatility and efficiency of the oxygen transport systems and nitrogen-fixation in biology

Learning Outcomes

After completion of the course the learners will be able to:
- Explain the electron transfer processes involving metal complexes
- Analyze the role of organometallics in catalysis and medicine and design new ones
- Analyze the structure and functions of metalloproteins
- Elaborate the oxygen transport system in various biosystems
- Illustrate the detoxification scheme for heavy metals and chelation therapy

UNIT I

Reaction mechanism- Labile, inert, stable and unstable complexes, classification of mechanisms- energy profile of reactions having different mechanisms.

Substitution in square planar complexes- factors affecting substitution, trans-effect, theories of trans-effect, application of trans-effect in the synthesis of complexes. Mechanism of ligand substitution in octahedral complexes- kinetics, factors affecting substitution in octahedral complexes: Leaving group, chelate and metal effects. Acid-Base catalysis: Acid catalysed aquation and anation reactions, base hydrolysis, conjugate base hydrolysis, stereochemistry of octahedral substitution, application of ligand substitution reactions for the synthesis of octahedral complexes.

A. Electron transfer reactions, complementary and non-complementary, outer sphere electro transfer- Marcus equation, Inner sphere electron transfer- one and two electron transfer, use of electron transfer reactions for the synthesis of complexes.

B. Oxidative addition, reductive elimination, isomerisation, migratory insertion reactions.

C. Metal ligand interactions with DNA.

UNIT II

Organometallics in Catalysis and Medicine: Basic principles, Isoelectronic and isolobal analogy, industrial requirements of catalysts. Homogeneous catalysis: Hydrogenation, asymmetric hydrogenation; hydrosilation- Chalk-Harrod mechanism: hydrocyanation- synthesis of buta-1,3-diene; hydroformylation- Cobalt and modified catalysts, Rh catalysts

Wacker process- acetaldehyde from ethylene; Monsanto acetic acid process, cativa process, Tennessee Eastmann process- Acetic anhydride from methyl acetate.Olefin metathesis; water gas shift reaction; Oligomerization- Shell High Olefin process; alkene isomerisation. Fischer Tropsch Process; Ziegler Natta Polymerization- syndiotactic, isotactic polymers, living polymerization; ammonia synthesis; Anchored catalysis- merits, polymer and metal oxides as supports; catalytic converters.

Medicinal applications of organometallic complexes, Titanocene as anticancer drug and other relevant molecules.

UNIT III

Metalloproteins: Structure and functions of metalloproteins in electron transfer process- Cytochromes, ferridoxines- 2Fe-2S, Rieske centers, high potential iron proteins; 4Fe-4S, 3Fe-4S, 8Fe-8S and rubredoxin. Mitochondrial flow of electrons from NADH to oxygen, cytochrome C, Cytochrome C oxidase.

Metalloenzymes: Structure and reactivity- Zinc enzymes: carboxypeptidase, carbonic anhydrase, alcoholdehydrogenase. Cu enzyme: superoxide dismutase. Mo enzyme: Xanthine oxidase, nitrate reductase. Fe enzymes: catalase, peroxidise and cytochrome P-450. Vitamin B_{12}: Coenzyme: B_{12r}, B_{12s}, biochemical functions of cobalamins; Biomethylation, mutase activity.

UNIT IV

Metals in transport, fixation and medicine

Na^+/K^+ transport across cell membranes, ionophores, crown ethers, Na^+/K^+ pump. Iron storage and transfer- ferritin, transferrin and siderophores. Metal ion deficiency and treatment (Fe, Zn, Cu, Mn); toxicity of Fe, Cu, Heavy metals- As, Hg, Pb and Cd; detoxification; chelation therapy; Biological roles of Ca: Binding sites of Ca^{2+} in proteins, importance of Ca^{2+} in muscle contraction and in blood clotting process

Oxygen transport and oxygen uptake proteins- transport and storage of dioxygen; Heme proteins and oxygen uptake, structure and functions of haemoglobin and myoglobin, dioxygen binding, Bohr effect, Hill equation; Model complexes for dioxygen binding, non- porphyrin systems- hemerythrin and hemocyanin.

Photosynthesis and nitrogen fixation: Nitrogenase: structural aspects and functions, abiological nitrogen fixation. Photosynthesis: Chlorophyll- structural features, role of Mg^{2+}, Z scheme of photosynthesis-PSI and PSII.

Metal complexes as anticancer and antiarthritic drugs.

SUGGESTED TEXT BOOKS

1. The organometallic chemistry of transition metals; R. H. Crabtee; John Wiley, 3rd edition, 2001.
2. Organometallics; Vol 1 & 2; M. Bochmann, Oxford Chemistry Primers, Oxford University Press, 1994.
3. Catalytic chemistry; B. C. Gates; John Wiley and sons, 1992.
4. Applied Organometallic chemistry and catalysis; Robin whyman, Oxford Chemistry Primers, 2001
5. Reaction mechanism of inorganic and organometallic systems; J. B. Jordon, Oxford University Press 2nd edition, 1998.
6. Principles of Bioinorganic Chemistry; S. J. Lippard and J. M. Berg; Panima Pub.Corporation 1997.
7. Bioinorganic Chemistry - Inorganic Elements in the Chemistry of Life, W Kaim, 2nd Edition, Wiley
8. Inorganic Chemistry, 3rd Edition; Gary. L. Miessler and Donald. A. Tarr (2007).
9. Inorganic Chemistry; K. F. Purcell and J. C. Kotz, Saunders Company, 1977.
10. Bio-inorganic chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, Viva Books Pvt. Ltd 1998.

SUGGESTED REFERENCE BOOKS

1. F. A. Carey G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, Wiley Interscience, 2003.
2. C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, Prentice Hall, 2005.

Course Details			
Course Title: Applications of spectroscopy techniques to inorganic systems			
Course Code	**MSCHE4002E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

To enhance the understanding of vibrational spectroscopy and discuss some specific cases of ambidentate, multidentate ligands and multinuclear complexes

- To lay the foundations of Raman spectroscopy and photoacoustic spectroscopy
- To acquaint the students with the core concepts of photoelectron spectroscopy and NMR spectroscopy and discuss its application in inorganic chemistry
- To highlight the efficacy of ESR (Electron Spin Resonance) spectroscopy in elucidating the structure and properties of inorganic complexes and free radicals.
- To acquaint the students with thee less common techniues such asMossbauer spectroscopy, NQR and X-ray absorption spectroscopy

Learning Outcomes: After completion of the course the learners will be able to:

- Analyze the FTIR spectra of mononuclear and multinuclear metal complexes with multidentate and ambidentate ligands
- Apply Raman spectroscopy to elucidate the structure and bonding of inorganic systems including the IR inactive ones
- Use NMR and photoelectron spectroscopy to explains structure and bonding in inorganic ccompounds
- Determine the structure and bonding in paramgnetic complexes and free radicals using ESR spectroscopy
- Apply Mossbauer spectroscopy technique to explain the magnetic properties of iron and tin based compounds

UNIT-I

Vibrational spectroscopy: Vibrational spectra of diatomic, linear and bent triatomic, AB_3, AB_4, AB_5 and AB_6 molecules, spectra of metal complexes: Ammine, amido, Nitro, Nitrito, lattice water, aquo and hydroxo, carbonato, nitrato, sulphato and other acido complexes, cyano and nitrile complexes, cyanato and thiocyanato complexes, mono and multinuclear carbonyl complexes, nitrosyls, phosphines and arsines, ambidentate ligands, ethylenediamine and diketonato complexes

Raman spectroscopy: Resonance Raman Spectroscopy, Nonlinear Raman effects-Stimulated, hyper and inverse types, Lasers and their use in Raman spectroscopy

Photoacoustic spectroscopy: Basic description and applications

UNIT-II

Photoelectron spectroscopy: Basic principles- photoelectric effect, Koopman's theorem, XPS and UPS, spin-orbit coupling in core level spectra, applications of core level spectra-ESCA, chemical shift, Valence level spectra- n, and bands, Auger electron spectroscopy and applications, Electron energy loss spectroscopy- basic principles and applications to the study of solids

NMR spectroscopy of inorganic molecules: Proton NMR spectra of metal hydride complexesNMR spectra of nuclei other than hydrogen: ^{19}F, ^{31}P, ^{11}B NMR spectra of simple compounds, Proton/hydride interactions with ^{103}Rh, ^{183}W, ^{195}Pt and ^{207}Pb in metal complexes/organometallic compounds, Solid State NMR.

UNIT-III

Electron spin resonance spectroscopy: Basic principles, the position of ESR absorption, significance of 'g' factor, determination of 'g'factor. Electron-nucleus coupling (Hyperfine splitting). ESR spectrometer, electron-electron coupling, double resonance in ESR, ENDOR, ELDOR. Interpretation of ESR spectra and structure elucidation of organic radicals using ESR spectroscopy. Spin density and Mc Connell relationship. Spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, zero/non-zero field splitting, Kramer's degeneracy, application to transition metal complexes (having one to five unpaired electrons) including biological molecules and inorganic free radicals such as PH_4, F_2 and BH_3.

UNIT-IV

Mossbauer spectroscopy: Basic principles, isomer shift, quadrupole splitting and magnetic hyperfine interactions, application to the study of bonding and structures of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+} compounds.

NQR spectroscopy: NQR isotopes, electric field gradients, Nuclear Quadrupole coupling constants, Experimental techniques and applications

X-ray absorption spectroscopy: Near edge measurements and EXAFS

SUGGESTED BOOKS

1. Physical methods in Inorganic Chemistry, R.S. Drago, Affiliated East West Press Pvt. Ltd., New Delhi (1965).
2. Infrared spectra of Inorganic and Coordination Compounds, K. Nakamoto, Wiley Interscience, New York (1970).
3. Vibrational Spectroscopy: Theory and Applications, D.N. Sathyanarayana, New Age International Publishers, New Delhi (2000).
4. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana, Universities Press, Bangalore (2001).

Course Details			
Course Title: Advanced Inorganic Materials			
Course Code	**MSCHE4003E04**	**Credits**	4
L + T + P	3 + 0+ 1	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To acquaint students with advanced inorganic materials such as intercalation compounds, composites and liquid crystals
- To make students aware of the recent advances made in the field of inorganic materials
- To impart knowledge about the salient features of superconducting materials, nanomaterials and 3-D printing materials
- To give hands-on-training in synthesis and characterization of advanced materials and some analytical techniques

Learning Outcomes: After completion of the course the learners will be able to:

- Analyze the role of Adavnced Materials such as liquid crystals and composites in daily life of mankind
- Have knowledge of emerging new materials and keep himself/herself aware of the recent advances in the field
- Analyze the structure, functions and utility of superconducting materials, nanomaterials and 3-D printing materials
- Synthesize nanomaterials showing unsusual properties such as surface plasmon resonance (SPR), superparamagnetism and size dependent absorption/luminescence (or quantum confinement effects)

UNIT I

Advanced Inorganic Materials–I: *Intercalation Compounds:* Intercalation reactions- layered structure-graphite interlayer compounds (GILC), staging of graphite, TaS_2, Microporous materials – zeolites and zeolitic materials, $AlPO_4$- $GaPO_4$.

Fibres and Composites
Synthetic inorganic chains and polymers- zirconia and other fibre Classification, microscopic composites, dispersion strengthened, particle reinforced, Fibre-glass reinforced composites, metal-matrix, plastic-matrix composites, hybrid composites.
Amorphous Materials*:* Crystalline versus amorphous solids, glass formation, Prepararion techniques-meltspinning, sputtering, ion implantation, Structural models of amorphous materials, Properties of metglasses - mechanical, electronic and magnetic properties.
Liquid Crystals*:* Mesomorphic behaviour, classification, examples - thermotropic and lyotropic liquid crystals Calamitic, nematic phase A, B, smectic phase, chiral nematic phase and optical Properties of liquid crystals. Applications with special reference to display systems

UNIT II

Advanced Inorganic Materials -II
Superconducting Materials: Transition Temperature, Meissner– Ochsenfeld Effect, Type I Superconductors, Type II Superconductors synthesis and structure of high temperature super conductors; Oxyhalides, oxycarbonates, ladder cuprates copper free oxide superconductors ,boro carbides ,super conducting fullerides,

cuprates materials and related preparation methods, making of films of superconductor by electron-beam, sputtering etc.

Nanomaterials: Nanomaterials as low dimensional systems, classification into 2D, 1D and 0D systems. Stabilization of colloidal nanoparticles. Classification of nanomaterials based on their properties: Semiconductor nanoparticles: Quantum confinement effects, size dependent optical properties; Magnetic nanoparticles: superparamagnetism, SPIONs, Giant magnetoresistance (GMR). Plasmonic nanoparticles: surface plasmon resonance, Carbon based nanomaterials: carbon nanotubes, fullerenes, graphenes, carbon dots, electron emission from CNTs, conductivity and enhanced catalytic activity compared to the same materials in the macroscopic state, NanoComposites

3-D Printing of materials and devices: Furndamentals of 3D printing (additive manufacturing), Implications of 3D printing in chemicals and biological sciences, PDMS based microfluidic devices, 3D printing of Li-ion battery, hydrogels, bone replicate materials, calcium phosphate ceramics

UNIT III

Advanced Materials Lab and Analytical Techniques

1. Estimation of metal acetates using perchloric acid in glacial acetic acid medium
2. Separation of metal ions by paper chromatography/TLC
3. Estimation of Iron III by solvent Extraction
4. AAS Estimation of Cu, Fe and Ni
5. Flame photometric estimation of K, Na from soil extract sample
6. Synthesis of CdSe quantum dots and to understand quantum confinement effects in semiconductor nanoparticles
7. Synthesis of silver nanoparticles and to understand the phenomenon of surface plasmon resonance in these systems
8. Synthesis of magnetite nanoparticles and to understand the phenomenon of superparamagnetism
9. Synthesis of polymer-metal nanocomposites and its characterization
10. Preparation and quantitative analysis of inorganic complexes: (a). Mercurytetrathiocyanatocobaltate, (b) Preparation of pentamminechloro cobalt(III) chloride

SUGGESTED TEXT BOOKS

1. Electrochemical Methods- Fundamentals and Applications, 2ndEdn, by A J Bard andL R Faulkner, John Wiley & Sons Inc., New York (2001).
2. Modern Electrochemistry, Vol.1, 2A and 2B by Bockris and Reddy, Plenum, N.Y (2000).
3. Magnetochemistry, R.L. Carlin, Springer Verlag.
4. Dana, M. Spence, Evaluation of 3D Printing and Its Potential Impact on Biotechnology and the Chemical Sciences, Analytical Chemistry, (ACS)

Course Details			
Course Title: Dynamic Stereochemistry, Reagents and Organic Synthesis			
Course Code	**MSCHE4004E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

OBJECTIVE: Utilise the knowledge of stereochemistry to understand different stereocontrolled chemical reactions. To understand the role of reagents in organic transformation with their reaction mechanism. Development of knowledge for rational mechanism-based design of synthetic strategies for new and novel organic reactions.

UNIT I

Dynamic Stereochemistry: Fundamental of asymmetric synthesis: Introduction, Topocity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic), groups and face asymmetry, Cram's and Prelog's rules substitution and addition criteria. Prochirality nomenclature: Pro-R, Pro-S, Re and Si. Selectivity in synthesis: stereo specific reaction, stereo selective reactions-examples of addition, elimination, substitution and rearrangement reactions. Enantioselectivity and diastereoselectivity.

Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methodology of asymmetric synthesis: Classification of asymmetric reactions into substrate controlled, chiral auxiliary controlled, chiral reagent controlled and chiral catalyst controlled. Diastereoselective transformation.

Molecular dissymmetry and chiroptical properties: Linear and circularly polarised lights, circular birefringence and circular dichroism, ORD and CD curves, Cotton effect. The axial haloketone rule, octant diagrams, helicity, and Lowe's rule. Application of ORD and CD to structural and stereochemical problems.

UNIT II

Reagents in organic synthesis: Use of the following reagents in organic synthesis and functional group tansformations**.**

Aluminium *iso*-propoxide, NBS, LDA, DCC, DDQ, Corey-Chaykovsky reagent, Raney-Nickel, diazomethane, TMS-chloride, 1,3-Dithiane (reactivity and umpolung), PPA, Yamaguchi reagent.

Oxidising Reagents: Oxidation: Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, aluminium, silver, and ruthenium. DMSO, hypervalent iodine and TEMPO based reagents). (b) phenols (Fremy's salt, silver carbonate) (c) alkenes to epoxides (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation.(d) alkenes to diols (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification, (e) alkenes to carbonyls with bond cleavage (Manganese, Osmium, Ruthenium and lead based, ozonolysis) (f) alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, selenium, chromium based allylic oxidation) (g) ketones to ester/lactones (Baeyer-Villiger).

Reducing Reagents: Reduction: (a) Catalytic hydrogenation (Heterogeneous: Palladium/ Platinum/ Rhodium/ Nickel etc; Homogeneous: Wilkinson). Noyori asymmetric hydrogenation. (b) Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium, Zinc, Titanium and Samarium (Birch, Pinacol formation, McMurry, Acyloin formation, dehalgenation and deoxygenations) (c) Hydride transfer reagents from Group III and Group IV in reductions. (i) $NaBH_4$ triacetoxyborohydride, L-selectride, K-selectride, Luche reduction; $LiAlH_4$, DIBAL-H, and Red-Al,; Trialkylsilanes and Trialkylstannane, Meerwein-Pondorff-Verley reduction) (ii) Stereo/enantioselectiviey reductions (Chiral Boranes, Corey-Bakshi-Shibata)

UNIT III

Organic Retrosynthesis and its application to natural product synthesis: Disconnection Approach: An introduction to synthons, retrons and synthetic equivalents, disconnection approach, the importance of the order of events in organic synthesis, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, illogical disconnections, linear and convergent synthesis. Chemo selectivity, regioselectivity, reversal of polarity (umpolung). Protecting Groups: principle of protection of important functional groups.

Functional group transposition, Functional group inter-conversions, Synthesis of some complex molecules: synthetic routes based on retrosynthetic analysis

SUGGESTED TEXT BOOKKS

1. F. A. Carey and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
2. M. B. Smith, Organic Synthesis, 2nd Edition, 2005
3. S. Warren, Organic Synthesis, The disconnection Approach, John Wiley & Sons, 2004.
4. J. Tsuji, Palladium Reagents and Catalysts, New Perspectives for the 21^{st} Century, John Wiley & Sons, 2003.
5. I. Ojima, Catalytic Asymmetric Synthesis, 2^{nd} edition, Wiley−VCH, New York, 2000.
6. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1996.
7. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2001.
8. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.
9. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.
10. Nasipuri D. Stereochemistry of Organic Compounds, New Age Publications.
11. Gawley R. E. and Aube J. Principles of Asymmetric Synthesis, Pergamon.
12. Eliel E. L. Stereochemistry of Organic Compounds, Wiley.

SUGGESTED REFERENCE BOOKKS

1. The Logic of Chemical Synthesis by E. J. Corey & X-M. Cheng
2. Classics in Stereoselective Synthesis by Carreira, E. M.; Kvaerno, L, Wiley VCH, 2009
3. Classics in Total Synthesis by K. C. Nicolaou & E. J. Sorensen, VCH, 1996.
4. Classics in Total Synthesis II, K. C. Nicolaou & S. A. Snyder, VCH, 2003.

Course Details			
Course Title: Medicinal, Combinatorial and Organomettalic reagents in Organic synthesis			
Course Code	**MSCHE4005E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

OBJECTIVE: To develop the basic understanding of the basic biological and pharmacological interactions by using both natural and synthetic bioactive molecules and use corresponding knowledge for the development of clinically active drugs. Get knowledge of the role of combinatorial chemistry in the drug discovery process. And finally understand the role of organometallic reagents in organic transformation with their reaction mechanism.

OUTCOME: At the end of this course students should be able to describe:
- The different targets and process to develope new drugs.
- The role of combinatorial chemistry in the drug discovery process
- The advantages of solid phase combinatorial synthesis
- Examples of resin beads used in solid phase synthesis
- The types of linkers employed in conjunction with solid supports
- The type of chemistry that can be employed on solid phase

UNIT I

Advanced Medicinal Chemistry: Drugs targets: Enzymes, receptors, nucleic acids and miscellaneous drug targets, pharmacodynamcs and pharmacokinetics.
Modern Drug discovery process: Market analysis, target selection, assay development.

Design and development: procedures followed in drug design, concepts of lead compound, lead modification: computer-aided design of lead compound, combinatorial and parallel synthesis, concepts of prodrugs and soft drugs.
Structure and activity Relationship (SAR), Drug optimization, Receptor Site Theory, Approaches to drug design. Factors affecting bioactivity, resonance, inductive effect, isosterism, bioisosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Computers in medicinal chemistry.
Pharmacokinetics: Absorption, Distribution, Metabolism and Excretion.
Illustration of drug development through specific examples: (a) Antibacterials: sulfonamides and penicillins (b) Antivirals: case studies with inhibitors of reverse transcriptase (nucleoside reverse transcriptase- and non-nucleoside reverse transcriptase inhibitors) and protease inhibitors. (c) Anticancer agents: antimetabolite-based approaches, those which affect signaling pathways or structural proteins such as tubulin

UNIT II

Combinatorial and Solid Phase Synthesis:

1. Introduction to Combinatorial Synthesis: Introduction; Merrifield synthesis of peptides; mix and split for combinatorial synthesis of peptides; deconvolution; orthogonal libraries;
2. Combinatorial Synthesis on the solid phase: Advantages; Resins: type and properties; Linkers; Selected Solid Phase Syntheses;
3. Combinatorial Synthesis in solution: Parallel synthesis; Indexed libraries; Dendrimers; Fluorous phase; impurity annihilation;
4. Encoded methods for Combinatorial Synthesis: Chemical tags; radio frequency tags; multiple release via orthogonal linkers;
5. Analytical techniques for Combinatorial Synthesis: On and off Bead analysis;
6. Solid supported reagents: Case studies - syntheses of carpanone and epibatidine.

UNIT III

Organometallic in Organic Synthesis: Application of the following organometallics in Organic Synthesis:
Organozincs: Preparation, reaction with compounds containing acidic protons, reaction with C-C multiple bonds, trans-metallation, addition reactions of zinc reagents with carbonyl compounds. Simmons Smith, and Reformatsky reaction. Organolithiums: Preparation. Deprotonation reactions, nucleophilic addition reactions, reactions with imines, nitriles and isonitriles.
Organocopper reagents: (Gilman reagents-lithium dialkyl cuprates): Preparation, reactions with alkyl, allyl, vinyl, benzyl and aryl halides, aldehydes, ketones

Organoseleniums: preparation. Use of organoseleniums in the synthesis of alkenes fromalkyl halides, α,β - unsaturated carbonyl compounds from carbonyl compounds. Organotelluriums: Debromination of vic-dibromides, deoxygenation of epoxides, oxidation of hydroquinone and synthesis of biaryls.
Organoaluminiums: Preparation, hydroalumination and carboalumination of alkenes. Nucleophillic addition reactions with carbonyl compounds and Hydrocyanation. Preparation of alkenyldialkylalanes and their reactions.
Organosilicons: Introduction, preparation and general reactions of trialkylsilyl halides. Peterson olefination.
Organotins: Preparation and reactions of tri-*n*-butyltin hydride, Barton decarboxylation and Barton-McCombie reaction.
Organocerates: Preparation and reactions of organocerates.

SUGGESTED TEXT BOOKS

1. Burger and Wolff M. E. Medicinal Chemistry and Drug Discovery, John Wile.
2. Pandeya S. S. & Dimmock J. R. Introduction to Drug Design, New Age International.

3. Graham & Patrick. Introduction to Medicinal Chemistry, OUP, 5th edition.
4. Goodman & Gilman. Pharmacological Basis of Therapeutics, McGraw-Hill.
5. Lednicer D. Strategies for Organic Drug Synthesis and Design, John Wiley

SUGGESTED REFERENCE BOOKS

1. Silverman, R. B., The Organic Chemistry of Drug Design and Drug Action. 2nd ed.; Academic Press: 2004.
2. Williams, D. A.; Lemke, T. L., Foye's Principles of Medicinal Chemistry. 5th ed.; Wolters Kluwer Health (India) Pvt. Ltd.: 2006.

Course Details			
Course Title: Spectroscopy and catalysis in Organic synthesis			
Course Code	**MSCHE4006E04**	**Credits**	4
L + T + P	2 + 1 + 1	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

OBJECTIVE: To develop an understanding of the basic principles of spectroscopy and to learn to apply these principles for structural elucidation of simple organic compounds. To build up a knowledge about the basic principle of catalysis in organic reactions.

UNIT 1

UV spectroscopy: Introduction, absorption laws, instrumentation, formation of absorption bands, types of electronic transitions, chromophores, auxochromes, absorption and intensity shifts, solvent effects, Woodward-Fieser rules for calculating absorption maximum in dienes and α–β-unsaturated carbonyl compounds.
IR spectroscopy: Introduction, theory of molecular vibrations, vibrational frequency, factors influencing vibrational frequencies, finger print region and applications of ir spectroscopy.

UNIT 2

Structure elucidation by NMR spectroscopy: Introduction, Magnetic properties of nuclei-Resonance condition, Nuclear spin, population of nuclear spin levels and NMR isotopes, Relaxation methods, Instrumentation; Classical approach.
Chemical shift, Factors influencing chemical shifts: electronegativity and electrostatic effects; Mechanism of shielding and deshielding in alkanes, alkyl halides, alkenes, aromatic compounds, carbonyl compounds and annulenes. Pascals triangle-low and high resolution, Reference compounds (internal and external reference compounds) Karplus Curve, Diamagnetic and Paramagnetic effects and Magnetic anisotropy. Equivalence of protons-chemical and magnetic equivalence; Spin systems: First order and second order coupling of AB systems, Simplification of complex spectra.
Spin-spin interactions: Homonuclear coupling interactions- AX, AX_2, AX_3, AMX, AB types. Vicinal, germinal and long range coupling-spin decoupling; Chemical shift reagents and deuterium exchange; reochemistry and hindered rotations. Temperature effects.
CIDNP, Nuclear Overhauser effect (NOE), Factors influencing coupling constants and Relative intensities.
Two-dimensional NMR spectroscopy, COSY, NOESY, DEPT and INEPT terminologies

^{13}**C NMR Spectroscopy**: Types of CMR spectra-undecoupled, proton decoupled, Off-resonance decoupled (SFORD); Selectively decoupled and gated decoupled spectra. ^{13}C chemical shifts of alkanes, alkyl halides, alkenes, alkynes, alcohols, ethers, carbonyl compounds and aromatic compounds; Factors affecting the chemical shifts. Applications of ^{13}C NMR spectroscopy in confirmation of structure and stereochemistry of organic molecules and in determining the reaction mechanism and dynamic processes of organic reactions –example Applications of NMR in organic chemistry as elucidation of structure of unknown compounds.

Mass Spectrometry: Introduction, ion production—EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, and ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, Molecular ion peak, Meta-stable peak, McLafferty rearrangement. Nitrogen Rule. High-resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination. Introduction to negative ion Mass spectrometry, TOF-MALDI. Problems based upon IR, UV, NMR and mass spectroscopy. Combined problems on UV, IR, NMR and Mass.

UNIT 3

Catalysis in Organic Reactions: Catalyst: Role of catalyst, general mechanism, Acid Catalysed Reaction, Base Catalysed Reaction, Nucleophilic catalyst, Metal-ion Catalysed Reaction, Intermolecular catalysis, Phase transfer catalysis, Organocatalysis, enzyme catalysed reactions

SUGGESTED TEXT BOOKS

1. Kemp, W. Organic Spectroscopy 3rd Ed., W. H. Freeman & Co. (1991).
2. Silverstein, R. M., Bassler, G. C. & Morrill, T. C. *Spectroscopic Identification of Organic Compounds* John Wiley & Sons (1981).
3. NMR Spectroscopy, H. Gunther, 2nd ed.; John Wiley and Sons, 1995

SUGGESTED REFERENCE BOOKS

1. Electron Paramagnetic Resonance of Transition Metal ions, A. Abragam, B. Bleaney, Oxford University Press, 1970.
2. Physical Methods for Chemist, R. S. Drago, Saunders, 1992.
3. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash, 4th ed, McGraw-Hill, 1994.
4. Spectroscopic methods in organic chemistry, D. H. Williams, I. Fleming, Tata McGraw Hill. 1988.

UNIT 4

Organic Chemistry Practical-IV:

(A) Preparations of various organic compounds employing different reactions such as

1. Diels-Alder reaction between furan and maleic acid,
2. Thiamine hydrochloride catalyzed benzoin condensation,
3. Pechmann consensation for coumarin synthesis,
4. Electrophilic aromatic substitution reaction,
5. Radical Coupling reaction,
6. Three component coupling reaction et.c

Products should be characterization using UV, IR and NMR technique with a view to give the student sufficient training in synthetic organic chemistry.

(B) Use of ultrasound and microwaves in organic synthesis
(C) Application of phase transfer catalysis in organic synthesis

Course Details			
Course Title: Advanced Quantum Mechanics and Surface Chemistry			
Course Code	**MSCHE4007E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

Students proficient in various methods such as Heitler-London method, HF-SCF-LCAO To acquaint students with advanced level concepts in quantum mechanics

- To make method etc.
- To make students aware of various advanced level concepts in surface chemistry such as Hertz-Knudsen equation, Langmuir-Rideal mechanism, Rideal-Eley mechanism etc.
- To make students learn methods to determine surface structure such as Harkins-Jura method, radioactive tracer method and Benton and White method
- To impart knowledge about instrumental techniques such as SEM, TEM. STM and AES for surface analysis

Learning Outcomes: After completion of the course the learners will be able to:

- Apply the concept and write quanum mechanical equations for simple molecules such as H_2, H_2^+ etc.
- Write expressions in terms of wave functions for hybrid orbitals, localized and delocalized molecular orbitals in polyatomic moleceules
- Determine the rate and entropy of adsorption
- Determine the surface structure using different instrumental techniques.

UNIT-I

QUANTUM CHEMISTRY-I: Theories of valence: Introductory aspects: Linear and non-linear variation functions. Secular equations. Coulombic, exchange, normalization and overlap integrals. Secular determinants. Molecular orbital (MO) theory, LCAO-MO approximation, application to Hydrogen molecule ion (H_2^+), energy levels of H_2^+, bonding and antibonding molecular orbitals, electron distribution, potential energy diagrams, comparison of theoretical and experimental values of energy. Valence bond (VB) theory of H_2molecule, the Heitler-London method, energy levels, energy distribution. Various modifications of the Heitler-London wave function.

Comparison of MO and VB theories. Ionic terms, fractional ionic characters and its importance, Equivalence of simple MO and VB methodsion-covalent resonance and configuration interaction. LCAO treatment of diatomic molecules, LCAO forms of simple wave function and molecular orbitals. Notations of molecular orbitals: full notation, Mulliken notation. MO configuration of homo- and hetero-nuclear diatomic molecules. Molecular electric terms. Bond order, stability and magnetic behavior of molecules from M.O. diagrams, isoelectronic systems. Correlation diagrams, non-crossing rule.

UNIT-II

QUANTUM CHEMISTRY-II: The HF-SCF-LCAO method. Directed valence, hybridization, Expressions for hybrid orbitals in terms of wave functions of s and p orbitals and explanation of directed valences of sp, sp^2, and sp^3 hybrid orbitals. Hybridization involving d-orbitals, Localized and non-localized molecular orbitals in polyatomicmolecules (H_2O).

Huckel molecular orbital theory: Outline of the method including assumptions. Application to ethylene, allylrdical, cyclopropenyl radical, butadiene, cyclobutadiene, bicyclobutadiene and benzene. Calculation of delocalization energy, charge density, π-mobile bond order and free valence.

UNIT-III

SURFACE CHEMISTRY-I

A. Review of adsorption curves, Adsorption-desorption, Adsorption forces, Heat of adsorption- Types, Measurements of heat of adsorption (Calorimetric and Clausius Clapeyron method), Measurement of adsorption isotherms, (Volumetric and Gravimetric methods), Determination of entropy of adsorption,
B. Electrostatic adsorption, adsorption indicators and their applications. Volcanic curves. Applications of adsorption.
C. Adsorption kinetics: Kinetics of chemisorption (Hertz-Knudsen equation), Chemisorptive bond, Competitive adsorption, Mechanism of some catalyzed surface reactions, Kinetic effects of surface heterogeneity, Kinetic effects of interactions, Potential energy curves for adsorption, Transition state theory of surface reactions, Rates of desorption, Kinetics of bimolecular surface reactions, Langmuir-Hinshelwood Mechanism, Langmuir-Rideal mechanism, Rideal-Eley mechanism and their comparison.

SURFACE CHEMISTRY-II

D. Adsorption theories: Polanyi's potential theory and Polarization theory. Hysteresis Of adsorption.
E. Surface structure: Surface mobility, Surface heterogeneity, Surface area and its determination by point-B method, Harkins-Jura method, radioactive tracer method and Benton and White method. Importance of surface area. Examination of surfaces by Interferometer method, Scanning electron microscopy (SEM), Low energy electron diffraction method (LEED method), Field Emission spectroscopy, Auger electron spectroscopy(AES), STM, and TEM.

SUGGESTED TEXT BOOKS

1. Molecular Quantum mechanics, P.W. Atkins and R.S. Friedman, Oxford University press (1997).
2. Introductory Quantum Chemistry by A. K. Chandra, Tata McGraw Hill (1994).
3. Quantum Chemistry by R.K. Prasad, 3rd Edn, New Age International (2006).
4. Quantum Chemistry by Ira N. Levine, Prentice Hall, New Jersey (1991).
5. Quantum Chemistry by Donald A McQuarrie, Viva Books Pvt. Ltd.New Delhi, India, Published in arrangement with Unversity Science books, Sausalito, CA, USA (2003).
6. Physical chemistry of surfaces by A. W. Adamson, Interscience Publishers Inc., New York (1967).
7. Surface Chemistry: Theory and Applications by J.J Bikertman, Academic Press, New York (1972).
8. Chemical Kinetics by K.J Laidler, 3rd Edn., Harper International Edn., (1987).
9. Text Book of Physical Chemistry by S. Glasstone, McMillan India Ltd. 2nd Edn. (1986).
10. Physical chemistry, R J Silbey, R. A. Alberty and M G bawendiEdn, Willey (2009).
11. Physics at surfaces, A Zangwill, Cambridge University Press (1988).
12. Surface crystallography, L J Clarke, Wiley-Interscience (1985).

Course Details			
Course Title: Applied Electrochemistry			
Course Code	**MSCHE4008E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To acquaint students with applications of electrochemistry in daily life
- To make students proficient in advanced level electroanalytical methods such as polarography and cyclic voltametry
- To make students aware of various methods of electrochemcical energy conversion and storage.
- To make students learn techniques of electroplating and metal finishing
- To impart knowledge about corrosion and its prevention

Learning Outcomes: After completion of the course the learners will be able to:

- Apply the concept of polarography and voltammetry to solve problems in daily life
- Explain the construction and working of various types of batteries and fuel cells
- Distinguish between various electroplating techniques and use it for different purposes
- Use electrochemical techniques to prevent corrosion

UNIT-I

APPLIED ELECTROCHEMISTRY

Electroanalytical methods: Voltametry: Definition, concentration polarization, ideal and non-ideal polarized electrodes, Faradaic and non-faradaic currents.

Polarography- Construction of dropping mercury electrode (DME), advantages and limitations. Principle of normal dc polarography, half-wave potential, and qualitative analysis using polarograms. Types of currents obtained at a DME. Ilkovic equation, factors affecting diffusion controlled current, quantitative analysis based on Ilkovik equation. current-potential relation for a cathodic wave, anodic wave and composite wave,test for the reversibility of a process at DME, factors that set the sensitivity and selectivity limits in normal dc polarography.

Advanced polarographic techniques: Tast polarography, normal pulse polarography, differential pulse polarography, ac polarography.

Stripping voltametry: Hanging drop mercury electrode (HDME), principles and applications of cathodic and anodic stripping voltammetry.

A: Cyclic voltammetry: Principle, experimental setup, qantitative analysis.Diagnostic criteria for reversible, quasi-reversible and irreversible processes.Study of coupled chemical reactions like E_rC_r, C_rE_r and $E_rC_iE_r$.

B. Chronomethods: Basic concepts, methodology and applications of chronoamperometry, chronopotentiometry and chronocoulometry.

C. Hydrodynamic electrodes: Construction and use of rotating disc and rotating ring disc electrodes in the electrochemical studies.

D. Membrane electrodes: Ion-selective membrane electrodes-construction and applications of solid state and liquid membrane electrodes, ion selective field effect transistor and Molecular (gas) sensing probes.

E. Problems solving.

UNIT-II

Electrochemical energy conversion and storage

Batteries: History and basics, classification, characteristics with units-voltage, current,capacity, electricity storage density, energy density, power density, energy efficiency, cycle life, shelf life. Primary batteries: Construction, reactions and uses of Leclanche' dry cell, alkaline Leclanche cell, zinc-silveroxide cell.

Secondary batteries: Construction, working (charge-discharge reactions), applications advantages and of Pb-acid and Ni-Cd batteries.

Hybrid Batteries: Metal-air batteries- meaning, Zn-air battery, Fe-air battery, Charging of metal- air battery, Metaloxide-hydrogen/hydride batteries, advantages and limitations of these cells *Lithium batteries:* Primary and secondary lithium battery,Li-ion battery and Lithium ion- polymer battery.

Electrochemical supercapacitors: comparative meaning of capacitor, electrolytic (super) capacitor and ultracapacitors, materials for construction, applications, advantages and limitations.
Fuel cells: Energy efficiency of electrochemical and thermal conversion (Carnot limitation).Definition of fuel cell, classification.Fuel cell efficiency- thermodynamic, electrochemical, practical efficiency.Electrode (anode and cathode) mechanism of fuel cell, Brief description on construction, working principle and applications of each type fuel cells. An account of electrocatalysts, proton exchange membrane (PEM) fuel cells anddirect methanol fuel cell. Problems solving.

UNIT-III

Surface Modification techniques (Metal finishing): Definition, important processes of metal finishing, technological importance of metal finishing. *Electroplating:* Definition, theory and mechanism of electroplating, effect of plating variables on the properties of electrodeposits, comparative account of complexing and non-complexing baths(general treatment), additives in the plating bath and their significance.

Metallic coating: Preparation of substrate surface, electroplating of Cu and Cr. Applications of Au and Ag platings.
Solar selective coatings: Characteristics, methods of preparation and applications.
Techniques of electroplating: Galvanizing, Anodizing, Phosphating, Chromating. Electroless plating: Definition, advantages over electroplating, pretreatment of substrates, an account of electroless plating of Ni including applications.

UNIT-IV

Corrosion and its Prevention
Introduction, dry and wet corrosion, theories and mechanisms of wet (electrochemical) corrosion, thermodynamic aspects of corrosion, kinetic aspects- determination of rates of corrosion by linear polarization, Tafel extrapolation and impedance techniques. Factors influencing the rate of corrosion- metal and environmental.
Methods of corrosion prevention: Cathodic protection, anodic protection, use of corrosion inhibitors, use of organic coatings.
Passivity: Definition, corrent potential diagram, characteristics of passivity, theory and mechanism of passivation, flade potential, trans passivity, Use of ellipsometric technique in the study of passivating films. Problems solving

SUGGESTED TEXT BOOKS

1. Modern Electrochemistry, Vol.1, 2A and 2B by Bockris and Reddy, Plenum, N.Y (2000).
2. Polarography and Allied Techniques by V SuryanarayanaRao, Universities Press (india) Pvt. Ltd.,
4. Hyderadad (2002).
3. Basic concepts of Analytical Chemistryby S M Khopkar, New Age Internatonal Publishers, third edition,
5. New Delhi, 2008.

4. Electroc hemical Methods- Fundamentals and Applications, 2nd Edn, by A J Bard and L R Faulkner, John Wiley & Sons Inc., New York (2001).
5. Chemical and Electrochemical Energy systems by Narayan and Viswanathan, Hyderabad, Universities Press (india) Pvt. Ltd., Hyderadad (2002).
6. Understanding Batteries, RM Dell and DAJ Rand, 2001.6. Fuel cells and their applications, Karl kordesh, gunter, Simader, VCH-Weinheim, Cambridge,1996.
7. Fundamentals of electrochemical deposition, Milan Paunovic and Mordechay
6. Schlesinger, Wiley- interscience publications, New York, 199
7. Electrodeposition and Corrosion Control, J. M. West, J. Wiley W. Revie (ed.): Corrosion Handbook, Electrochemical Society Series, John Wiley and Sons (2000)
8. Electrochemistry and corrosion science, Nestor Perez, Springer pvt. Ltd., 2004
9. Principles and Prevention of Corrosion, D. A. Jones, Macmillan Publ. Co. (1996).
10. Bioelectrochemistry: Fundamentals, experimental techniques and application, P. N. Bartlett, Wiley& Sons (2008).
11. Synthetic organic Electrochemistry by A M Fry, 2nd Edn, Wiley 1989.

Course Details			
Course Title: Lasers in Chemistry			
Course Code	**MSCHE4009E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Even	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

To acquaint the students with the fundamentals of lasers and its use in chemistry

- To make students aware of different types of laser sources such as, solid state lasers, He-Ne Lasers, Exciplex lasers etc,
- To make students learn how lasers are integrated and used in some well-known analytical techniques such as chromatography, polarimetry etc.
- To make students learn the application of lasers in driving photochemical reactions and in inducing therapeutic effects such as photodynamic and photothermal therapy
- To develop an understanding of laser-based spectroscopy techniques such as Laser Stark Spectroscopy, Absorption Spectroscopy, Laser Magnetic Resonance, Fluorescence Spectroscopy etc.

Learning Outcomes

After completion of the course the learners will be able to:

- Distinguish between coherent and non-coherent light sources
- Explain the basic concepts involved in making and working of lasers
- Discuss the salient features of various lasers such as semiconductor lasers, exciplex lasers, solid state, molecular gas lasers etc
- Explain how advent of lasers have enhanced the efficacy of various analytical techniques such as chromatography, polarimetry etc.
- Examine and evaluate the relevance of lasers in daily life such as its use in photochemical reactions and photodynamic/photothermal therapy
- Underscore the importance of laser-based spectroscopic techniques

UNIT I

Operation of Laser

The Nature of Stimulated Emission, Resonators and Pumping Processes, Coherent Radiation, Standing Waves and Modes, The Kinetics of Laser Emission: Rate Equations, Threshold Conditions, Pulsed Versus Continuous Emission; Transitions, Lifetimes and Linewidths: Three-level Laser, Four-level Laser, Emission Linewidths; Properties of Laser Light, and Their Applications: Beamwidth, Coherence, Intensity, Monochromaticity

UNIT II

Laser Sources

Solid-state Transition Metal Ion Lasers: Ruby Laser, Neodymium Lasers; Semiconductor Lasers, Atomic and Ionic Gas Lasers: Helium-neon Laser, Argon Laser, Copper Vapour Laser; Molecular Gas Lasers: Carbon Dioxide Laser, Nitrogen Laser, Chemical Lasers, Iodine Laser, Exciplex Lasers; Dye Lasers, Free-electron Lasers

UNIT III

Laser Instrumentation in Chemistry

Polarising Optics, Frequency Conversion, Pulsing Techniques: Cavity Dumping, Q-Switching, Mode-locking; Detectors, Pulse Detection Systems: Lock-in Amplifiers, Boxcar Integrators, Single-pulse Systems; Light

Scattering Instrumentation: Nephelometry, Photon Correlation Measurements, Brillouin Scattering, Doppler Velocimetry, Lidar; Polarimetry, Laser Detectors in Chromatography, Laser Microprobe Instrumentation

UNIT III

Laser-Induced Chemistry

Principles of Laser-induced Chemistry: Multiphoton Infra-red Excitation, Reaction Rates and Yields; Laser Photochemical Processes: Unimolecular Laser-induced Reactions, Bimolecular Laser-enhanced Reactions, Laser-sensitised Reactions, Laser Surface Chemistry, Ultrafast Reactions, Laser Reaction Diagnostics; Isotope Separation: Photo ionisation, Photo dissociation, Photochemical Reaction, Photo deflection; Miscellaneous Applications: Purification of Materials, Production of Ceramic Powders, Photodynamic and Photothermal therapy

UNIT IV

Spectroscopy with Lasers

Absorption Spectroscopy, Specialised Absorption Techniques: Excitation Spectroscopy, Ionisation Spectroscopy, Thermal Lensing Spectroscopy, Photo acoustic Spectroscopy, Optogalvanic Spectroscopy, Laser Magnetic Resonance,
Laser Stark Spectroscopy; Fluorescence Spectroscopy: Laser-induced Atomic Fluorescence, Laser-induced Molecular Fluorescence; Raman Spectroscopy

SUGGESTED TEXT BOOKS

1. D. L. Andrews, Lasers in Chemistry, Springer, Heidelberg
2. S. Chopra, Lasers in Chemical and Biological Sciences, New Age International Publishers (1992).
3. H. H. Telle, A. G. Ureña, R. J. Donovan, Laser Chemistry: Spectroscopy, Dynamics and Applications, Wiley publications (2007)
4. M. Lackner, Lasers in Chemistry, Vol. I & Vol. II., Wiley VCH (2008).

Course Details			
Course Title: Green Energy Systems			
Course Code	**MSCHE4010E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To make students aware of the emerging energy scenario with respect to fast depletion of fossil fuels and climate change
- To impress upon the students the need to innovate and design cleaner and greener techniques to generate energy
- To develop a thorough understanding of nuclear reactors and its use for power generation
- To make students learn the principles, design and working of electrochemical power sources
- To impart the knowledge about fuel cells and emphasize the importance of hydrogen as a fuel
- To develop a comprehensive understanding of solar cells

Learning Outcomes: After completion of the course the learners will be able to:

- Understand the energy crisis in relation to climate change
- Compare and contrast the green and non-green energy sources
- Explain how nuclear reactors are used for power generation
- Distinguish between primary and secondary electrochemical power sources
- Discuss the relevance of hydrogen as green fuel
- Explain the working of various types of solar cells

UNIT I

Overview of energy scenario: Available energy options, their advantages and disadvantages. Environmental effects, comparative evaluation of energy options and energy needs. Fossil fuels: petroleum, natural gas and coal Origin, processing and production of value added products available current conversion technologies.

UNIT II

Nuclear Energy: Nuclear Energy: Principles of Fission, Fission reactors, U enrichment and processing of spent fuels. Nuclear reactor kinetics and control nuclear fusion magnetic and other confinement evaluation of the option of nuclear energy.

UNIT III

Electrochemical Cells: Electrochemical power sources theoretical background on the basis of thermodynamic and kinetic considerations.
Primary cells- various types, especially magnesium and aluminium based cells, magnesium reserve batteries. Secondary cells: classification based on electrolyte type, temperature of operation on the basis of electrodes, chemistry of the main secondary batteries for electric vehicles- present status.

UNIT IV

Hydrogen as fuel: Fuel cells: classification chemistry of fuel cells detailed description of hydrogen/oxygen fuel cells methanol molten carbonate solid polymer electrolyte and biochemical fuel cells. Hydrogen as fuel production (thermal, electrolysis, photolysis and photo electrochemical) storage and applications of hydrogen storage.
Solar energy conversion devices, photovoltaic cells, photo electrochemical cells, dye sensitized solar cells, semiconductor/electrolyte junctions, photocatalytic modes for fuel conversion process, photo biochemical options.
Other methods of energy conversion: processes especially in the form of storage as chemical energy.

SUGGESTED TEXT BOOKS

1. C. A. Vincent Modern Batteries, Edward Arnold, 1984.
2. R. Narayanan and B. Viswanathan, Chemical and Electrochemical energy systems, Orient Longmans, 1997.
3. K. Sriram, Basic Nuclear Engineering, Wiley Eastern, 1990.
4. A. S. J. Appleby and F. K. Foulkes, Fuel cell Hand Book, Von Nostrand Reinhold, 1989.
5. D. Linden, Hand book of batteries and Fuel cells, McGraw Hill Book Company, 1984.
6. T. Ohta, Solar Hydrogen energy systems, Peragamon Press, 1979.
7. M. Gratzel, Energy Resources through photochemistry and catalysis, Academic Press, 1983.
8. T. Ohta, Energy Technology, Sources, Systems and Frontiers conversions, Pergamon, 1994.
9. J. G. Speight, The chemistry and technology of petroleum, Marcel Dekker Inc. (1980).

Course Details			
Course Title: Advanced Instrumental Techniques-II			
Course Code	**MSCHE4011E04**	**Credits**	4
L + T + P	3 + 1 + 0	**Course Duration**	One Semester
Semester	Odd	**Contact Hours**	45 (L) + 15 (T) Hours
Methods of Content Interaction	Lecture, Tutorials, Group discussion; self-study, seminar, presentations		

Course Objectives

- To equip the students with necessary skills in advanced instrumental techniques
- To make students proficient in various electroanalytical techniques such as cyclic voltammetry, coulometry, pulse polarography etc.
- To impart skills in thermal methods of analysis
- To make students learn the chemical composition analysis using different instrumental methods
- To acquaint students with different types of microscopy techniques such as SEM, TEM, STM, AFM, MFM, CT, OCT etc

Learning Outcomes

After completion of the course the learners will be able to:

- Apply electoanalytical techniques such as voltammetry, polaraography etc for physicochemical analysis
- Analyze thermal stability of materials and compounds using techniques such as TGA, DTA, DSC
- Determine the chemical composition of compounds/materials using CHN, XRF, ICP-AES techniques
- Perform the microstructural analysis using microscopy techniques such as SEM, TEM, AFM, STM etc.

UNIT-I

Electroanalytical Techniques: Electrode Potential, Currents in Electrochemical cells, Potentiometric titrations. Electrogravimetry-faraday's laws of electrolysis, Coulometry, Coulometric titrations. Voltammetry- principle, DME-advantages, limitations, HydrodynamicVoltammetry, Cyclic voltammetry-priciple, conditions for reversible, quasi reversible and irreversible reactions. Anodic stripping voltammetry-priciple and applications, Polarography, Pulse polarography, Amperometry-titrations, different titration curves,applications, numerical problems on all these techniques .

UNIT-II

Thermal Methods of Analysis: Principle, methodology and applications: thermogravimetric and differential thermal analysis, differential scanning calorimetry; Thermo-mechanical and dynamic mechanical analysis; thermometric titrations. Thermal stability of polymers, applications, decomposition patterns, decomposition reactions-examples.

UNIT-III

Chemical Composition Analysis: CHN Analysis, Atomic absorption spectroscopy, Inductively Coupled Plasma-Atomic Emission spectroscopy (ICP-AES), X-ray fluorescence (XRF) technique.

UNIT-IV

Microscopy & Imaging Techniques: Scanning Probe Microscopy: AFM, STM, MFM, Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), STEM, 23 Vibrational Imaging: IR, Raman, CARS, SRS, X-ray Microscopy and Micro-Computed Tomography (CT) , Optical Coherence Tomography (OCT)

SUGGESTED TEXT BOOKS

1. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt, and J. A. Dean, 6th Edition (1986),
2. Quantitative Chemical Analysis, Daniel C. Harris
3. Spectrometric Identification of Organic Compounds, 7th Edition, Robert M. Silverstein, Francis X. Webster, David Kiemle.
4. William Kemp, Organic spectroscopy, Pal grave, New York.
5. Introduction to Spectroscopy. Donald L. Pavia, James A. Vyvyan.
6. Fundamentals of Analytical Chemistry by A. Skoog and M. West
7. Vogel's Hand Book of Quantitative Analysis by Longman
8. Physical methods for chemists: R.S. Drago

SUGGESTED REFERENCE BOOKS

9. R. Wiesendanger, Scanning Probe Microscopy and Spectroscopy, Cambridge University Press, 1994.
10. Frank A. Settle, Handbook of instrumental techniques for analytical chemistry, Prince Hall, New Jersey, 1997.
11. K. W. Kolasinski, Surface science: Foundations of catalysis and nanoscience, John Wiley and Sons, West Susses, 2002.
12. D. A. Skoog, D. M. West, F. J. Holler and S. R. Couch, Fundamentals of analytical chemistry. Brooks/ColeCengage learning, New Delhi, 2004.
13. P. Atkins and J. de Paula, Atkins' physical chemistry, 8th Ed., Oxford University Press, New Delhi, 2008.
14. T. Pradeep, Nano: The essentials, McGraw-Hill Education, New Delhi, 2010.
15. F. Scholz, Electroanalytical Methods, Springer, 2nd Ed., 2010.