MSc. Chemistry (2 Years)

CURRICULUM AND SYLLABUS

(Effective from 2018 Admission Onwards)

Vision of the Institute

To be a global leader in the delivery of engineering education, transforming individuals to become creative, innovative, and socially responsible contributors in their professions.

Mission of the Institute:

1. To provide best-in-class infrastructure and resources to achieve excellence in technical education,
2. To promote knowledge development in thematic research areas that have a positive impact on society, both nationally and globally,
3. To design and maintain the highest quality education through active engagement with all stakeholders –students, faculty, industry, alumni and reputed academic institutions,
4. To contribute to the quality enhancement of the local and global education ecosystem,
5. To promote a culture of collaboration that allows creativity, innovation, and entrepreneurship to flourish, and
6. To practice and promote high standards of professional ethics, transparency, and accountability

PROGRAM OUTCOMES (PO)

Students of all Integrated/PG degree Programmes at the time of graduation will be able to

PO1. **Science knowledge**: Knowledge of basic science fundamentals

PO2. **Problem analysis**: Develop analytical skills to identify, formulate, analyze complex mechanisms using first principles basic sciences.

PO3. **Development of solutions**: Design solutions for complex chemical process problems and evolve procedures that meet the specified needs with appropriate consideration for the public health and safety and environmental considerations.

PO4. **Critical review of solutions:** Use of research-based knowledge and research methods including design of experiments, analysis and interpretation of data, and synthesis of the information to provide valid conclusions.

PO5. **Modern analytical tool usage**: Select, and apply appropriate techniques, resources, and modern analytical tools

PO6. **The scientist and society**: Apply reasoning through the contextual knowledge to assess societal, health, safety, legal and cultural issues and the consequent responsibilities relevant to the professional chemical practice.

PO7. **Environment and sustainability**: Understand the impact of the chemical processes in societal and environmental contexts, and demonstrate the knowledge of, and need for sustainable development.

PO8. **Ethics**: Apply ethical principles and commit to professional ethics and responsibilities and norms of the chemistry practice.

PO9. **Individual and team work**: Function effectively as an individual, and as a member or leader in diverse teams, and in multidisciplinary settings.

PO10. **Communication**: Communicate effectively on complex scientific activities with the science community and with society at large, such as, being able to comprehend and write effective reports and design documentation, make effective presentations, and give and receive clear instructions.

PO11. **Project management and finance**: Demonstrate knowledge and understanding of the scientific and management principles and apply these to one's own work, as a member and leader in a team, to manage projects and in multidisciplinary environments

PO12. **Life-long learning:** Recognize the need for, and have the preparation and ability to engage in independent and life-long learning in the broadest context of technological change

PROGRAM SPECIFIC OUTCOMES (PSO)

PSO1: Graduate can demonstrate the understanding the basic principles of synthetic and analytical applications of chemistry along with proficiency in communication and professional excellence in project management and execution.

PSO2: Graduate will be competent for higher education in world class universities, research in industrial organizations and also to seek a career in teaching.

PSO3: Graduate can be employable in research and development, analytical and quality control services and also motivated for entrepreneurship.

PSO4: Graduate will manifest commitment to society, environmental awareness, moral and ethical values in scientific scenario.

MSc. Chemistry (2 Years)

CURRICULUM

(Effective from 2018 Admission Onwards)

SEMESTER I

Course Code	Course Title	L T P	Cr	ES
18CHY501	Quantum Chemistry	3 0 0	3	
18CHY505	Group Theory and its Applications	3 0 0	3	
18CHY502	Concepts in Inorganic Chemistry	3 1 0	4	
18CHY503	Principles in Organic Chemistry	3 0 0	3	
18CHY504	Coordination Chemistry	3 0 0	3	
18CHY581	Inorganic Semi-micro Qualitative Analysis Lab.	0 0 5	2	
18CHY582	Organic Quantitative Analysis Lab.	0 0 5	2	
18CUL501	Cultural Education	2 0 0	P/F	
	TOTAL		**20**	

SEMESTER II

Course Code	Course Title	L T P	Cr	ES
18CHY511	Chemical Thermodynamics and Equilibria	3 1 0	4	
18CHY512	Molecular Spectroscopy	3 1 0	4	
18CHY513	Organic Reaction Mechanism	3 1 0	4	
18CHY514	Heterocyclic and Natural Products Chemistry	3 0 0	3	
18CHY515	Organometallic Chemistry	3 0 0	3	
18CHY583	Advanced Physical Chemistry Lab.	0 0 5	2	
18CHY584	Inorganic Quantitative Analysis Lab.	0 0 5	2	
18AVP501	Amrita Value Programme	1 0 0	1	
	TOTAL		**23**	

SEMESTER III

Course Code	Course Title	L T P	Cr	ES
18CHY601	Electrochemistry, Kinetics and surface Chemistry	3 1 0	4	
18CHY602	Synthetic Strategies and Reagents	3 1 0	4	
18CHY603	Solid State Chemistry and Materials Science	3 0 0	3	
18CHY604	Bioinorganic Chemistry	3 0 0	3	
	Elective	3 0 0	3	
18CHY681	Organic Qualitative Analysis Lab.	0 0 5	2	
18CHY682	Instrumental and Analytical Methods Lab.	0 0 5	2	
18CHY690	Live-in-Lab.@ / Open Elective*	2 0 0	2	
	TOTAL		**23**	

SEMESTER IV

Course Code	Course Title	L T P	Cr	ES
18CHY696	Dissertation		14	
	TOTAL		**14**	
	TOTAL	**80**		

Electives

Course Code	Course Title	L T P	Cr	ES
18CHY631	Applied Electrochemistry	3 0 0	3	E
18CHY632	Bioanalytical Chemistry	3 0 0	3	E
18CHY633	Chemistry of Biomolecules	3 0 0	3	E
18CHY634	Industrial Chemistry	3 0 0	3	E
18CHY635	Industrial Stoichiometry	3 0 0	3	E
18CHY636	Material Science and Nanochemistry	3 0 0	3	E
18CHY637	Medicinal Chemistry	3 0 0	3	E
18CHY638	Supramolecular Chemistry	3 0 0	3	E
18CHY639	Nanomaterials for Biomedical Applications	3 0 0	3	E
18CHY640	Industrial Metal Finishing Processes	3 0 0	3	E
18CHY641	Biosensors: Fundamentals and Applications	3 0 0	3	E
18CHY642	Computational Chemistry	3 0 0	3	E
18CHY643	Sustainable Chemical Science	3 0 0	3	E

Open Electives

Course Code	Course Title	L T P	Cr
18OEL631	Advanced Statistical Analysis for Research	2 0 0	2
18OEL632	Basics of PC Software	2 0 0	2
18OEL633	Computer Hardware and Networking	2 0 0	2
18OEL634	Consumer Protection Act	2 0 0	2
18OEL635	Corporate Communication	2 0 0	2
18OEL636	Design Studies	2 0 0	2
18OEL637	Disaster Management	2 0 0	2
18OEL638	Essentials of Cultural Studies	2 0 0	2
18OEL639	Foundations of Mathematics	2 0 0	2
18OEL640	Foundations of Quantum Mechanics	2 0 0	2
18OEL641	Glimpses of Life through Literature	2 0 0	2
18OEL642	Information Technology in Banking	2 0 0	2
18OEL644	Knowledge Management	2 0 0	2
18OEL645	Marketing Research	2 0 0	2
18OEL646	Media for Social Change	2 0 0	2
18OEL647	Media Management	2 0 0	2
18OEL648	Object-Oriented Programming	2 0 0	2
18OEL649	Painting and Sculpture	2 0 0	2
18OEL650	Personal Finance	2 0 0	2
18OEL651	Principles of Advertising	2 0 0	2
18OEL652	Principles of Packaging	2 0 0	2
18OEL653	Scripting for Rural Broadcasting	2 0 0	2
18OEL654	Social Media Website Awareness	2 0 0	2
18OEL655	Theatre Studies	2 0 0	2
18OEL656	Writing for Technical Purposes	2 0 0	2
18OEL657	Yoga and Personal Development	2 0 0	2
18OEL658	Fundamentals of Legal Awareness	2 0 0	2
18OEL659	Solid Waste Management and Utilization	2 0 0	2
18OEL660	Relativistic Quantum Mechanics	2 0 0	2
18OEL661	Robotics and Biology	2 0 0	2
18OEL662	Science of Well Being	2 0 0	2
18OEL663	Operating Systems and Networks	2 0 0	2
18EN600	Technical Writing	2 0 0	2
18OEL664	Bhagavat Geeta and Personality Development	2 0 0	2
18OEL665	Chemical Aspects of Forensic Science	2 0 0	2

* **Two Open Elective** courses are to be taken by each student, one each at the **4th and the 5th** semesters, from the list of Open electives offered by the School.

[@] Students undertaking and registering for a Live-in-Lab project, can be exempted from registering for an Open Elective course in the fifth semester

Evaluation Pattern

50:50 (Internal: External) (All Theory Courses)

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
*Continuous Assessment (CA)	20	
End Semester		50

80:20 (Internal: External) (Lab courses and Lab based Courses having 1 Theory hour)

Assessment	Internal	External
*Continuous Assessment (CA)	80	
End Semester		20

70:30(Internal: External) (Lab based courses having 2 Theory hours/ Theory and Tutorial)

Theory- 60 Marks; Lab- 40 Marks

Assessment	Internal	External
Periodical 1	10	
Periodical 2	10	
*Continuous Assessment (Theory) (CAT)	10	
Continuous Assessment (Lab) (CAL)	40	
End Semester		30

65:35 (Internal: External) (Lab based courses having 3 Theory hours/ Theory and Tutorial)
Theory- 70 Marks; Lab- 30 Marks

Assessment	Internal	External
Periodical 1	10	
Periodical 2	10	
*Continuous Assessment (Theory) (CAT)	15	
Continuous Assessment (Lab) (CAL)	30	
End Semester		35

*CA – Can be Quizzes, Assignment, Projects, and Reports.

Letter Grade	Grade Point	Grade Description
O	10.00	Outstanding
A+	9.50	Excellent
A	9.00	Very Good
B+	8.00	Good
B	7.00	Above Average
C	6.00	Average
P	5.00	Pass
F	0.00	Fail

Grades O to P indicate successful completion of the course

$$CGPA = \frac{\sum (C_i x Gr_i)}{\sum C_i}$$

Where

C_i = Credit for the i^{th} course in any semester

Gr_i= Grade point for the i^{th} course

Cr. = Credits for the Course

Gr. = Grade Obtained

Sc. Chemistry (2 Years)

SYLLABI

(Effective from 2018 Admission Onwards)

18CHY501 QUANTUM CHEMISTRY 3 0 0 3

Course Outcomes

CO1: Thorough understanding of the fundamentals of quantum chemistry
CO2: Capability to provide innovative solutions (in the language of quantum chemistry) for problems of chemical interest.
CO3: Development of familiarity with computational techniques and tools which finds extensive applications in practical quantum chemistry
CO4: Become convinced about the greenness of the theoretical methods in chemistry

Unit I: Quantum Chemistry - Introduction
Origin of quantum mechanics, de Broglie relationship, the uncertainty principle (no derivation); Postulates of quantum mechanics: postulate I – wave functions, postulate II- Operators in quantum mechanics, operator algebra, postulate-III – eigen values, eigen value equations, postulate IV – Expectation value, postulate V – time dependent and time independent Schrodinger equation

Unit II: Applying Schrodinger equation to various general systems
Translational motion of a quantum entity (particle in one dimensional box and three dimensional box); vibrational motion (harmonic oscillator); rotational motion (rigid rotator, particle on a ring and particle on a sphere); angular momentum.

Unit III: Atomic structure and chemical bonding
Hydrogen and hydrogen-like atoms; Multi electron systems- variation methods, perturbation methods, application to the ground state of Helium atom, SCF method, the exclusion principle
Chemical bonding: Hydrogen molecule ion and hydrogen molecule - molecular orbital and valence bond theory, homo and hetero nuclear diatomic molecules from VB and MO theory, the concept of directed valences and hybridization; quantum mechanics in band theory of metallic solids

Unit IV: Electronic structure of polyatomic systems: Computational quantum chemistry
Semi empirical and ab-initio methods; QM approximations, **Details of HMO and EHMO** and its application to chemical bonding in unsaturated molecules(ethylene, 1,3butadiene etc) ; Details of SCF procedure, Hartree and Hartree Fock methods (up to ground and excited states of hydrogen molecule); the basis sets, STOs and GTOs, nomenclature of basis sets, basis set errors, introductory ideas on DFT.

Unit V: Molecular properties: Computational quantum chemistry

Calculations of molecular properties like atomic charges, dipole moments, electronic distributions, vibration frequencies, NMR chemical shift etc using Gaussian program, specification of molecular geometry using Cartesian coordinates and internal coordinates, Z-matrix, Z-matrix of some simple molecules, structure of a Gaussian input file

TEXTBOOKS:

1. *Ira N. Levin, 'Quantum Chemistry', 6th Edition, Prentice-Hall, 2008*
2. *Peter Atkins, Ronald Friedman, 'Molecular Quantum Mechanics', 4th edition, Oxford university press*
3. *R K Prasad, 'Quantum Chemistry', New Age International (P) LTD publishers*

REFERENCES:

1. *Andrew R Leech,' Molecular Modeling – Principles and Applications', 2nd Edition, Pearson Education.*
2. *Donald A. McQuarrie, 'Quantum Chemistry', Viva Books 2016.*

18CHY505 GROUP THEORY AND ITS APPLICATIONS 3 0 0 3

Course Outcomes

CO1: Development of sound knowledge on fundamentals of group theory as applied in chemistry

CO2: Ability to apply group theory in various applied and allied areas of chemistry (such as spectroscopy and chemical bonding.

CO3: Development of capability to utilize the principles of group theory to provide innovative solutions for problems of chemical interest.

Unit I Introduction to molecular point groups

Definition of a mathematical group, Symmetry in molecules, elements of symmetry, , matrix representation of symmetry operations, molecular point groups, , abelian group, cyclic group, symmetry operations as group elements, similarity transformation and classes, group multiplication table, symmetry classification of molecules into pointgroups (Schoenflies symbol)

Unit II Construction and interpretation of character tables

Reducible and irreducible representations, Great Orthogonality Theorem and its consequences, character tables, reduction formula, construction of character tables for point groups with order ≤6, interpretation of character tables.

Unit III Applications of Group theory - I (vibrational and electronic spectroscopy)

Infrared and Raman activity of molecular vibrations in H_2O, N_2F_2, BF_3, AB_4type molecules (Td and D_4h) and AB_6 type (Oh) of molecules; selection rules; Electronic structure of free atoms and ions, splitting of terms in a chemical environment, construction of energy level diagrams,

estimations of orbital energies, selection rules and polarizations, double groups, a brief idea on electronic spectra of transition metal complexes – selection rules, Orgel diagrams, Tanabe Sugano diagrams.

Unit IV: Applications of Group theory (Chemical bonding - Hybridization and molecular orbital formation)

Group theory to explain hybridization - wave functions as bases for irreducible representations, construction of hybrid orbitals for AB_3 (planar), AB_4 (Td), AB_5 (D_{3h}) and AB_6 (O_h) type of molecules, symmetry adapted linear combinations, projection operators, application of projection operators to pi-bonding in ethylene, cyclopropenyl systems and benzene, application of symmetry to predict polar and chiral compounds;

Unit V: Symmetry in solid state

Symmetry elements and operations in solid state – proper axis of rotation, mirror planes of symmetry, roto- reflection and roto-inversion axes of symmetry, screw axes of symmetry, glide planes; a brief introduction to the crystallographic point groups and space groups

TEXTBOOKS:

1. *F.Albert Cotton, 'Chemical Applications of Group Theory', 3rd Edition, John Wiley, 1990.*
2. *A Salahuddin Kunju, G Krishnan ; 'Group theory and its application in chemistry', second edition, PHI Learning private limited-2015*

REFERENCES:

1. *Robert L Carter, 'Molecular symmetry and Group theory', John Wiley & Sons, Inc.*
2. *V.Ramakrishnan and M.S.Gopinathan, 'Group Theory in Chemistry', 2nd reprint edition, Vishal Publications, 1996.*
3. *P.H.Walton, "Beginning Group Theory for Chemistry", Oxford University Press Inc., New York, 1998.*

18CHY502 Concepts in Inorganic Chemistry 3 1 0 4

Course Outcomes

CO1: Capacity to describe the structure of nucleus, stable and unstable atomic nuclei, nuclear reactions and different modes of radioactive decay, kinetics of nuclear reactions

CO2: Ability to understand the fundamentals of radiochemistry, isotopic chemistry, radiation chemistry and the applications of these in measuring technology, kinetics, radical chemistry, biotechnology and methods for measurements of radioactivity.

CO3: Capacity to distinguish the structure, bonding and reactivity of clusters, cages and simple organometallic compounds of alkali, alkaline earth elements, boron and carbon.

CO4: Impeccable understanding in structure and reactivity of inorganic chains, rings and cages of sulfur, nitrogen and phosphorus compounds

CO5: Capability to demonstrate the basic knowledge of chemistry of the f-block elements. Both chemical and physical properties of these elements and their compounds, with an emphasis on the relationship between properties and underlying electronic structure

Unit 1 Nuclear Chemistry

Nuclear structure, mass and charge, mass defect, binding energy, stability rules, magic numbers, nuclear quantum numbers, nuclear parity and statistics, models of nucleus, shell model, liquid drop model, , semi empirical mass equation, equations of radioactive decay and growth, half-life, average life determination of half-lives, nuclear reactions, energetics of nuclear reactions, types of nuclear reactions, spontaneous and induced fission, neutron capture cross sections- critical size principle and working of nuclear reactor. Numerical problems relevant to each session.

Unit 2 Radiation Chemistry

Radioactive elements, decay kinetics, parent-daughter decay relationships, radioactive equilibrium - transient and secular equilibrium, alpha and beta decay, gamma emission, Radiochemical methods - measurement of radioactivity, measurement of radiations - ionization chamber, proportional counter, the Geiger counter, scintillation counter, semiconductor detectors. Applications of nuclear and radiation chemistry, isotope dilution analysis - activation analysis, radioactive tracers, radiometric titrations, radiation dosimetry, hydrated electron.

Unit 3 Inorganic materials I

Alkali and alkaline earth metals, their compounds, crown ethers and cryptands as complexing agents for alkali metal ions, Be and Mg compounds, boron cage compounds, boron hydrides, structure and bonding, 3-centre-2-electron bonds, styx numbers, the importance of icosahedral frame work of boron atoms in boron chemistry, closo, nido and arachno structure, carboranes, metallocene carboranes, B-N compounds, interstitial compounds, metal carbides, nitrides and hydrides, fullerenes, functionalized fullerenes, C-nanotubes .

Unit 4 Inorganic materials II

Inorganic chains and polymers, rings, cages, and clusters, sulphur-nitrogen compounds, polymeric sulphur nitride, isopoly anions, heteropoly anions, Keggin and Dawson polyoxometallates, borazines, metal clusters, nature of Si-Si bonds, silicates, silicates with zero-, one-, two- and three-dimensional structures, structure of elemental P, phosphonitrilic compounds, polymers with P-N bonds, interhalogen and pseudo halogens, intercalation chemistry, intercalation in layered materials like graphite, xenon fluorides & other xenon compounds.

Unit 5 Chemistry of f-block elements

The lanthanides and actinides, stable oxidation states, the lanthanide and actinide contractions, the f-orbitals, spectral and magnetic properties - comparison with inner transition and transition metals, separation of lanthanides, use of lanthanide compounds as shift reagents, photo-emission

of lanthanide compounds, organometallic compounds of lanthanides and actinides and their structural features, reactions of lanthanide and actinide compounds, mineral sands of south west India - Ilmenite, Monazite, etc.

TEXTBOOKS:

1. H J Arnikar, Essentials of Nuclear Chemistry, 4th revised edition, New Age International (P) Limited publishers, 2015.
2. H J Arnikar, Nuclear Chemistry through Problems, New Age International Publishers.
3. J. Huheey, Inorganic Chemistry: Principles of Structure and Reactivity, 4th edition, 2006.
4. F.A. Cotton, Advanced Inorganic Chemistry, Wiley; 6th Edition edition (22 April 1999)
5. J.D. Lee Concise Inorganic Chemistry, Oxford University Press, 5th edition, 2008

REFERENCES:

1. Gregory R. Choppin, Jan-Olov Liljenzin and Jan Rydberg, Radiochemistry and Nuclear Chemistry (Third Edition), Elsevier, 2002
2. Walter D. Loveland, David J. Morrissey, Glenn T. Seaborg, Modern nuclear chemistry, A JOHN WILEY & SONS, INC., PUBLICATION, 2017.
3. **Shriver and Atkins' Inorganic Chemistry, Oxford; 5 edition, 2009**

18CHY503 Principles in Organic Chemistry 3 0 0 3

Course Outcomes

CO1: Be able to understand the concepts of aromaticity and field effects
CO2: Understand and reproduce accepted mechanisms of organic reactions including all intermediates, arrows, charges, and resonance structures.
CO3: Be able to draw all the stereoisomers of organic compound and recognize enantiomers, diastereomers, mesocompounds
CO4: Discuss the relative stability of conformational isomers of cyclohexanes and related compounds
CO5: Predict the major and minor products of a variety of organic reactions with appropriate stereochemistry and regiochemistry.

Unit 1 Aromaticity: Review of inductive and field effects – Resonance effects. Criteria for aromaticity – structural and electronic. Types – Huckel and Craig's rule, homo (Five, Six, seven and eight, membered rings), hetero (furan, thiophene and pyrrole) and nonbenzenoid aromatic systems. Aromaticity of fused rings, annulenes, catenanes, rotaxanes, mesoionic compounds, metallocenes, cyclic carbocations and carbanions.

Unit 2 Structure activity relationships – Orientation effects of substituent, Quantitative treatment of structure on reactivity - free energy relationships – Hammet equations, Taft equation.
Reactive Intermediates: Generation, structure and reactivity - reactions and rearrangement involving) of carbocations - non-classical carbocations, carbanions, carbon radicals, radical ions, carbenes, nitrenes, isonitrenes, arynes.

Unit 3 Mechanism and methods to determining them: Thermodynamic and kinetic requirement, Baldwin rules for ring closure – Kinetic and thermodynamic control – Hammond postulates, microscopic reversibility, Marcus theory, methods of determining reaction mechanisms - solvents and their effect on course of a reaction.
Acids and Bases: Bronsted and Lewis acids - HSAB concept and bases, pH and pKa, effect of structure on acidity and basicity, effect of medium.

Unit 4 Stereochemistry
Optical and geometrical isomerism, absolute and relative configuration, Cahn-Ingold-Prelog system, prochirality, prochiral centre, atoms, groups and faces, designations. Atropisomerism, optical isomerism in biphenyls, allenes, spirans and "ansa" compounds, compounds containing chiral nitrogen and sulfur atom, geometrical isomerism of cyclic compounds, cumulenes and oximes. Asymmetric synthesis, stereospecific and stereoselective synthesis, regioselective and regiospecific reactions.

Unit 5 Conformational Analysis
Conformational analysis of cyclic and acyclic systems with special emphasis on six membered rings, conformational effects on the reactivity of acyclic and cyclic systems - elimination, substitution and addition, strain, structure and stability of small, medium, and large rings, anomeric effect - cycloalkenes and cycloalkynes - kinetically and thermodynamically favoured products stereochemistry of SN1, SN2, SNi, E1 and E2
Selectivity in organic reactions: Chemoselectivity, regioselectivity, enantio- and stereo-selectivity. Stereoaspects of the addition of X_2, HX, boranes and hydroxylation to C=C systems. *Cis*- and *trans*- hydroxylation of cycloalkenes.

TEXT BOOKS

1. Michael B Smith, "March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure", 7th edition, Wiley (2015).
2. Francis A.Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part A: Structure and Mechanisms", 5th Edition, Springer, 2008
3. P. S. Kalsi, "Stereochemistry, Conformation and Mechanism", New Age Publications, 2008.

REFERENCES

1. E. L. Eliel and S. H. Wilen, "Stereochemistry in Organic Compounds", John Wiley, 2008.

2. D. Nasipuri, "Stereochemistry of Organic Compounds - Principles and Applications", 4th Revised Edition, New Academic Science, 2012.
3. Peter Sykes, "A Guidebook to Mechanism in Organic Chemistry", Pearson Education; 6 edition, 2003.

18CHY504 Coordination Chemistry 3 0 0 3

Course Outcomes

CO1: Understanding the nature of bonding in co-ordination complexes

CO2: Acquiring wide knowledge of reaction mechanism, stereochemistry, thermodynamic and kinetic stability of the octahedral and square planar complexes

CO3: Indispensable knowledge about the coordination behavior, shape, geometry, oxidation state, stereochemistry and reaction mechanism of f-block elements.

CO4: Developing the skill in analyzing the electronic spectra of transition metal complexes.

CO5: Acquiring the knowledge of magnetic properties of metal complexes and the recent advancement in the coordination complex based magnets.

Unit 1 Theories and Concepts on *d*-block Coordination Compounds

Introduction - ligands, nomenclature of coordination compounds, coordination compounds of *d*-block ions with coordination numbers of 2, 3, 4, 5, 6, 7 and 8. Werner's coordination theory, Valence bond theory (VBT), Crystal field theory (CFT), CFSE, effects of CFSE on hydration energies and spinel groups (normal and inverse), types of ligands – spectrochemical series, spectral and magnetic properties (spin-only magnetic moments), nephelauxetic effect. Crystal field splitting patterns in complexes having Oh, Td, square planar, square pyramidal and trigonal pyramid geometries, factors affecting the magnitude of CFSE, various types of isomerism in coordination complexes, Jahn-Teller (JT) distortion, manifestation of JT on spectral properties. Molecular orbital theory (MOT), ligand field theory (LFT), molecular orbital energy level diagram for octahedral complexes without pi-bonding, metal-ligand pi-bonding, metal-metal multiple bonds, *d*-orbital based metal-metal σ, π and δ bonds in compounds like $[Re_2Cl_8]^{2-}$, $[Os_2Cl_8]^{2-}$, $Cr_2(CH_3COO)_4$ and R-Cr(I)-Cr(I)-R. Application of group theory to coordination compounds.

Unit 2 Reaction Mechanism

Complex equilibrium - formation constants, chelate and macrocyclic effects, factors affecting stability of complexes, methods of determination of stability constants, stability of complex ions in solutions, inert and labile complexes, mechanisms of ligand displacement and addition

reactions in octahedral complexes and square planar complexes of platinum *cis*- and *trans*-effect, substitution reactions, mechanisms of substitution, kinetic consequences of reaction pathways, dissociation, interchange, association, dissociation, linear free energy relationships, conjugate base mechanism, stereochemistry of reactions (substitution in *trans*-complexes and substitution in *cis*-complexes), isomerisation of chelate rings, sigma-bonding and pi-bonding effects, oxidation-reduction reactions, inner and outer sphere electron transfer reactions, conditions for high and low oxidations numbers, reactions of coordinated ligands, hydrolysis of esters, amides and peptides, template reactions, electrophilic substitution, photochemical reactions of coordination compounds.

Unit 3 Coordination Chemistry of Inner-transition (*f*-block) Elements

f-block metal ions – oxidation states preferences, ligand preferences, coordination numbers and the geometry of the complexes, influence of lanthanide contraction and actinide contraction in their coordination behaviour, shapes of *f*-orbitals (4*f* and 5*f*), nature of bonding of *f*-orbitals with ligands, various types of coordination compounds of lanthanides and actinides, stereochemistry and reaction mechanism of *f*-block metal complexes.

Unit 4 Spectral Properties

Stabilization of unusual oxidation states, electronic spectra of transition metal complexes – color wheel, Russell-Saunders coupling schemes, term symbols for various d^n ions, Orgel diagrams for d^n systems, ligand field parameters, *Dq*, Racah parameter *B* and nephelauxetic constant *b*, Tanabe-Sugano (TS) diagrams, evaluation of *Dq* and other parameters from electronic spectra of transition metal complexes using TS diagrams, charge-transfer transitions, MLCT and LMCT, selection rules and band intensities, Laporte- and spin- selection rules, symmetry, spin-orbit and vibronic coupling effects. Photochemistry of transition metal complexes like $[Ru(bipy)_3]^{2+}$, spectral behaviour of *f*-block coordination complexes, special features of their absorption and emission properties.

Unit 5 Magnetic Properties

Magnetic properties of coordination complexes - magnetic susceptibility, contribution of spin-orbit coupling on μ_{eff}, types of magnetic behavior - para-, ferro, anti-ferro and ferri-magnetic systems, Curie law, Curie-Wise law, Guoy, Faraday and superconducting quantum interference device (SQUID) methods, Kotani plots, giant magnetoresistance (GMR), anisotropic magnetoresistance (AMR) effect, effects of temperature on magnetic behavior, tunnelingmagnetoresistance (TMR). Magnetism of coordination complexes by multinuclear homo- and heterometallic 3*d* systems (also with exclusive 4*d* and 5*d* metal ions), mixed 3*d*-4*f* systems, importance of 4*f*-metal ions for functional applications. Nanoscale magnetic systems based on coordination complexes - Single Molecule Magnets (SMMs), Single Ion Magnets (SIMs), Single Chain Magnets (SCMs), Spin-crossover complexes, magnetic refringents (magnetic coolers), magnetic storage systems - magnetic random access memory (MRAM).

TEXTBOOKS:

1. F. A. Cotton and G. Wilkinson, 'Advanced Inorganic Chemistry', John Wiley & Sons, 2009.

2. James E. Huheey, Ellen A. Keiter and Richard L.Keiter, 'Inorganic Chemistry, Principles of Structure and Reactivity', Pearson education, 5th edition, 2009.
3. J. D. Lee, 'Concise Inorganic Chemistry', 5th edition, John Wiley & Sons, 2009.
4. P Atkins, T. Overton, J. Rourke, M.Weller, F. Armstrong, "Shriver & Atkins Inorganic chemistry", 4th Edition, Oxford University Press, 2008.

REFERENCES:

1. B. Douglas, D. McDaniel and J. Alexander "Concepts and Models in Inorganic Chemistry", 3rd Edition, Wiley, 2006.
2. SushantaDattagupta, 'A Paradigm Called Magnetism', World Scientific Publishing Co. Pte. Ltd., 2008.
3. Helen C. Aspinall, 'Chemistry of the *f*-Block Elements', Volume 5 of Advanced chemistry texts, CRC Press, 2001.
4. N. N. Greenwood and A. Earnshaw, 'Chemistry of Elements', Butterworth and Heinemann, 2nd Edition, 2002
5. J. E. House, "Inorganic Chemistry", Academic Press, 2008.
6. T. Shinjo (Editor), 'Nanomagnetism and Spintronics', Elsevier, USA, 2nd Ed., 2014.
7. R. A. Layfield and M. Murugesu (Editors), 'Lanthanides and Actinides in Molecular Magnetism', Wiley-VCH Verlag& Co., 2015.

18CHY581 INORGANIC SEMI-MICRO QUALITATIVE ANALYSIS LAB 0 0 6 2

Course Outcomes

CO1: Development of skill to perform classical qualitative analysis of cations in a mixture of inorganic salts/compounds.

CO2: Development of adequate knowledge of the chemistry involved in the cation analysis.

CO3: Attainment of knowledge and skill in activities related with effective and safe functioning of a chemistry lab.

Semi micro analysis of mixtures

The mixture will include 4 cations including two common (eg. Cations of metals like Cu, Mn, Zn, Ni, Ca, Ba, Mg etc) and two less common cations (eg. Cations of metals like Ti, Zr, V, W, Li, Ce, Th etc).

(The student has to successfully analyze a minimum of 10 mixtures).

TEXTBOOKS:

1. *A.I.Vogel, 'A text book of Qualitative Analyses', 4th edition, Longmans publications, 1985.*
2. *V.V. Ramanujam, 'Inorganic Semi-Micro Qualitative Analysis', 3rd edition, The National Publishing Company, 1974.*

REFERENCES:

1. *G.H.Jeffery, J.Bassett, J.Mendham and R. C. Denney, 'Vogel's Text Book of Qualitative Chemical Analysis', 5th edition, John Wiley & Sons Inc, 1989.*
2. *G.W. Parshall, 'Inorganic Synthesis', Vol. 15, Tata McGraw-Hill Education, 1974.*

18CHY582 Organic Quantitative Analysis Lab 0 0 6 2

Course Outcomes

CO1: Understanding in calculation of limiting reagent, yield, and percent yield. Also, ability to summarize findings in a clear and concise manner.

CO2: Actively engage in safe laboratory practices handling laboratory glassware, equipment, and chemical reagents including how to perform common laboratory techniques, including reflux, distillation, steam distillation, recrystallization, vacuum filtration, aqueous extraction, thin layer chromatography, column chromatography.

CO3: Wide knowledge in prediction of outcome and mechanism of some simple organic reactions, using a basic understanding of the relative reactivity of functional groups.

CO4: Basic knowledge in basic characterization of organic molecules by physical and spectroscopic means, including melting point, boiling point, Infrared red spectroscopy and NMR.

CO5: Capability to estimate the amount of organic compounds

A. Estimations: 1. Estimation of equivalent weight of an acid 2. Estimation of glucose 3. Estimation of phenol 4. Estimation of acetone 5. Estimation of acid value of an oil 6. Estimation of iodine value and sap value of an oil 7. Estimation of Nitrogen – Kjeldahl method 8. Estimation of formaldehyde 9. Estimation of aniline 10. Estimation of ester
B. Preparations of Organic Compounds Double stage preparations (a) m-nitro benzoic acid from ethyl benzoate (b) p-bromobenzanilide from aniline (c) p-nitro acetanilide from aniline Single stage preparations (a) Benzimidazole (b) Benzophenone oxime (c) Dibenzilidene acetone (chalcone) (d) Benzalacetophenone (e) Benzanilide (f) Acetanilide (g) Acetyl salicylic acid (aspirin)

Name Reactions (a) Benzil-Benzilic acid rearrangement (b) Cannizaro reaction (c) Claisen condensation

For all preparations 1. TLC to be done and Rf values of each compound to be reported 2. Melting point of pure compounds to be found 3. A small portion should be recrystallised from suitable solvent 4. Purified products to be displayed 5. Mechanisms for each preparation should be suggested

REFERENCES:

1. P.W.G. Smith, A.J.Hannaford, B.S.Furnis and A.R. Tatchell, "Vogel's Textbook of Practical Organic Chemistry", ELBS/Logman, 1989.
2. Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill, David Y. Curtin, Reynold C. Fuson, 'Systematic Identification of Organic Compounds', John Wiley & Sons, 2003.
3. Mann and Saunders, 'Practical Organic Chemistry', Pearson edition, 2009

18CUL501 CULTURAL EDUCATION 2 0 0 2

Objective:

Love is the substratum of life and spirituality. If love is absent life becomes meaningless. In the present world if love is used as the string to connect the beads of values, life becomes precious, rare and beautiful like a fragrant blossom. Values are not to be learned alone. They have to be imbibed into the inner sprit and put into practice. This should happen at the right time when you have vitality and strength, when your hearts are open.

The present course in value education is a humble experience based effort to lead and metamorphosis the students through the process of transformation of their inner self towards achieving the best. Amma's nectarous words of wisdom and acts of love are our guiding principles. Amma's philosophy provides an insight into the vision of our optimistic future.

1. Invocation, Satsang and Question - Answers
2. Values - What are they? Definition, Guiding Principles with examples Sharing own experiences
3. Values - Key to meaningful life. Values in different contexts
4. Personality - Mind, Soul and Consciousness - Q and A. Body-Mind-Intellect and the Inner psyche Experience sharing
5. Psychological Significance of samskara (with eg. From Epics)
6. Indian Heritage and Contribution and Q and A; Indian Ethos and Culture
7. Self Discipline (Evolution and Practice) – Q and A
8. Human Development and Spiritual Growth - Q and A
9. Purpose of Life plus Q and A
10. Cultivatingself Development
11. Self effort and Divine Grace - their roles – Q and A; - Vedanta and Creation - Understanding a spiritual Master
12. Dimensions of Spiritual Education; Need for change Lecture – 1; Need for

Perfection Lecture - 2

13. How to help others who have achieved less - Man and Nature Q and A, Sharing of experiences

REFERENCES:

1. Swami AmritaswaroopanandaPuri - Awaken Children (Volume VII and VIII)
2. Swami AmritaswaroopanandaPuri - Amma's Heart
3. Swami RamakrishnandaPuri - Rising Along the Razor's Edge
4. Deepak Chopra - Book 1: Quantum Healing; Book 2: Alpha and Omega of God; Book 3: Seven Spiritual Rules for Success
5. Dr. A. P. J. Abdul Kalam - 1. Ignited Minds 2. Talks (CD)
6. Swami RamakrishnandaPuri - Ultimate Success
7. Swami JnanamritanandaPuri - Upadesamritham (Trans: Malayalam)
8. Vedanta Kesari Publication - Values - Key to a meaningful life
9. Swami Ranganathananda - Eternal values for a changing society
10 David Megginson and Vivien Whitaker - Cultivating Self Development
11. Elizabeth B. Hurlock - Personality Development, Tata McGraw Hill
12. Swami Jagatatmananda - Learn to Live (Vol.1 and 2), RK Ashram, Mylapore

Course Outcomes:

CO1: Understanding Indian culture
CO2: Understanding Indian value system, Human Development and Spiritual Growth
CO3: Learn about Dimensions of Spiritual Education

18CHY511 CHEMICAL THERMODYNAMICS AND EQUILIBRIA 3 1 0 4

Course Outcome

CO1: Thorough understanding of the fundamental concepts in classical, statistical and irreversible thermodynamics as needed for a chemist.

CO2: Development of capability to apply the knowledge in thermodynamics to solve problems of chemical interest.

CO3: Utilize the acquired knowledge in thermodynamics to formulate innovative solutions for problems connected with applications in the field of chemistry and allied branches.

Unit 1 Chemical Thermodynamics

First and second laws of thermodynamics, thermodynamic functions, heat capacity, thermo chemistry, need for second law of thermodynamics, entropy and free energy functions, calculation of changes in thermodynamic function for ideal and non-ideal gases in isothermal and adiabatic process, relation between thermo dynamic functions - Maxwell relations, Joule Thomson effect, coefficient of thermal expansion and compressibility factor, applications of free energy function to physical and chemical changes, equilibrium in chemical reactions, third law of thermodynamics - need for third law, calculation of absolute entropy, unattainability of absolute zero, thermodynamic systems of variable composition - fugacity functions, partial molar quantities, thermodynamics of ideal solutions, real solutions and regular solutions, dilute solutions of nonelectrolytes, Henry's law, Raoult's law, Gibbs-Duhem equations, Gibbs-Duhem-Margules equations, and activity and standard states of non electrolytes.

Unit 2 Irreversible Thermodynamics

Examples for irreversible process, entropy production, non-equilibrium, steady state and near equilibrium conditions, linear relation, phenomenological coefficients, Onsagar reciprocal relations, one component systems with heat and matter transport, application of irreversible thermodynamics to thermal diffusion, thermal osmosis etc., electro kinetic effects, the Glansdorf-Pregogine equation.

Unit 3 Statistical Thermodynamics

Statistical concept, probability and thermodynamic states, entropy and probability, canonical ensemble, Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein Statistics, electron gas concept, Bose-Einstein condensation, relation among MB, FD & BE Statistics, partition function, partition function for free linear motion, free motion in a shared space, linear harmonic vibration, translational, rotational and vibrational partition function, molecular partition functions, partition functions and thermodynamic properties, calculation of equilibrium constant, heat capacity of gases, mono atomic solids, Einstein's and Deby's theory.

Unit 4 Equilibrium

Gibb's free energy, direction of spontaneous change of a reaction, chemical potential, chemical potential and equilibrium, ΔG in terms of K, equilibrium constants – real gases and real reactions, equilibrium respond to catalyst, temperature, pressure and $_{P}H$, application of ΔG and K – extraction of metals from their oxides, Ellingham diagram, and thermodynamics of ATP & respiration, biological energy conversion.

Unit 5 Phase Equilibrium

Gibb's Phase rule, one component system, two component systems, vapour pressure diagrams and their interpretation, lever rule, temperature-composition diagrams, liquid-liquid phase diagrams, distillation of partially miscible liquids, azeotropes, liquid-solid phase diagrams, phase diagram for the system Na/K/Na_2K, phase diagram - steel, alloys, Fe-C system, zone refining, three component system, triangular coordinates, three component system – partially miscible liquids - $H_2O/CHCl_3/CH_3COOH$, phase diagram - $NH_4Cl/(NH_4)_2SO_4/H_2O$

TEXTBOOKS:

1. Robert J. Silbey, Robert A. Alberty, Moungi G. Bawendi, Physical Chemistry 4th Edition, Wiley, 2004
2. Samuel H. Maron, Carl F. Prutton Principles of Physical Chemistry, The Macmillan Company; 4th edition (1970)
3. *Samuel Glasstone, 'Thermodynamics for Chemists', Lightning Source Incorporated, 2007.*

REFERENCES:

1. Francis Weston Sears and Gerhard L.Salinger, 'Thermodynamics, kinetic theory and statistical thermodynamics' 3rd edition, Addison-Wesley Publications, 1975.
2. Prigogine, 'Introduction to Thermodynamic Irreversible Processes', Interscience Publishers, 3rd edition, 1968.
3. R.P.Rastogi and R.R.Misra, 'An Introduction to Chemical Thermodynamics', 6th Revised edition, Vikas Publishing House Pvt. Ltd., 2006.
4. F.W.Sears, 'Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics', Addison Wesley Pub., Cambridge, 1972.

18CHY512 MOLECULAR SPECTROSCOPY 3 1 0 4

Course Outcomes

CO1: Thorough understanding of the fundamental theoretical concepts of spectroscopy, based on quantum chemistry, group theory and statistical thermodynamics.

CO2: Thorough understanding of the fundamentals of instrumentation of spectroscopic techniques.

CO3: Development of capability to apply the knowledge spectroscopy to provide analytical solutions for problems of chemical interest.

Unit 1 Rotational and Vibrational Spectroscopy

Introduction to spectroscopy, rotation spectra - diatomic and polyatomic molecules, selection rules, intensities of spectral lines, stark effect, instrumentation of micro wave spectroscopy, applications and structural determinations, vibration spectra of diatomic molecules, harmonic and anharmonic vibrations, diatomic vibrating rotor, selection rule, breakdown of Born Oppenheimer approximation, rotational character of vibration spectra, different modes of vibrations, vibration-rotation spectra, Fermi resonance, vibration spectra of polyatomic

molecules, IR spectra of organic and inorganic compounds, phase, temperature and solvent dependence, FTIR technique, instrumentation, Raman spectra (including the use of laser) - theory, relation with IR spectroscopy, mutual exclusion principle, resonance Raman, stimulated hyper and inverse Raman effects, instrumentation and applications of Raman spectroscopy.

Unit 2 UV-Visible and Fluorescence Spectroscopy

Electronic spectra of atoms - single and multi electron systems, j-j and L-S coupling, electronic spectra of diatomic and polyatomic molecules, its relation to electronic arrangement and symmetry of molecules, application of group theory in electronic spectra, selection rules, nature of electronic excitation, principles of absorption spectroscopy, Beer-Lambert law, presentation of spectra, chromophores, forbidden transition, different types of electronic transitions, p-p*, n-p* etc transitions, nature of transitions in carbonyl compounds, the effect of conjugation, effect of conjugation on alkenes, HOMOs and LUMOs, Woodward-Fieser rules for dienes, spectra of carbonyl compounds, enones, Woodward rule for enones, spectra of aromatic compounds, effect of substituents, structural information from electronic spectra, excited states of molecules, fluorescence and phosphorescence, Jablonski diagram in detail, lifetime of excited states, quantum yields, photosensitization, application of UV-Visible and Fluorescence Spectroscopy for structural elucidation of organic compounds, diffuse reflectance spectra.

Unit 3 NMR Spectroscopy

Nuclear magnetic resonance phenomenon - theory, relaxation effects, NMR uses active nuclei, Fourier Transformation in NMR, measurement of relaxation time, chemical shift, magnetic anisotropic effect, multiplets in NMR, spin-spin splitting, n + 1 rule, Pascal's triangle, tree-diagram, spin-spin splitting constant, J, ^{2}J and ^{3}J and long-range coupling, measurement of J, Karplus relationship, first and second order spectra, AX, AB, AX_2, AX_3, A_2X_3, AMX type spectra, double resonance and spin tickling, chemical shift reagents, spectra in higher fields, spectra of conformational isomers, homotopic, enantiotopic and diastereotopic systems, C^{13} spectra, factors related to ^{13}C spectra, ^{1}H coupled ^{13}C spectra, ^{1}H decoupled ^{13}C spectra, chemical shift values, nuclear Overhauser effect (NOE), cross-polarization, off-resonance resonance decoupling, application of ^{1}H and ^{13}C NMR spectroscopy for the structural elucidation of organic compounds, ^{11}B, ^{15}N, ^{19}F and ^{31}P NMR spectra, spectra of paramagnetic complexes, magnetic susceptibility, contact shift, fluxional molecules and their studies using NMR, solid state NMR.

Unit 4 ESR, NQR and Mossbauer Spectroscopy

ESR spectroscopy - theory, hyperfine and superfine splitting, ESR active simple organic systems, ESR of inorganic systems like Cu^{2+} and VO^{2+} complexes, 'g' markers like DPPH and TCNE, evaluation of spin Hamiltonian like A, g_{ll}, g-, covalency factor in Cu^{2+} complexes, analysis of ESR spectra of VO^{2+} complexes, NQR spectroscopy - theory, relationship between electric field gradient and molecular structure, quadrupole coupling constant and structural information of compounds, Mossbauer spectroscopy, principle, Doppler effect, isomer shift, Zeeman splitting, quadrupole splitting, application of Mossbauer spectroscopy for studying Fe and Sn compounds and phase transformation, application of ESR spectroscopy.

Unit 5 Mass Spectrometry and PES

Mass spectroscopy, base peak and molecular ion peak, isotope ratio data, fragmentation patterns of alkanes, alkenes, alkynes, aromatic hydrocarbons, alcohols, phenols, aldehydes, ketones, esters, carboxylic acids, amines, methods of desorption and ionization (EI, CI, LD, MALDI, PD, FAB, SIMS), MS/MS and determination of molecular formula, metastable ions and their significance, study of fragmentation pattern, application of MS in structural elucidation and other frontiers of science, application of MS for quantitative analysis, photoelectron spectroscopy (PES), principle, application of PES. Structure determination using IR, UV-visible, NMR, MS and ESR spectral techniques.

TEXTBOOKS:

1. *Colin N. Banwell and Elaine M. McCash, 'Fundamentals of Molecular Spectroscopy', 4th Edition, Tata McGraw Hill, 2007.*
2. *W. Kemp, Organic Spectroscopy, 3rd Edition, McMillan International Higher Education*
3. *D. L. Pavia, G. M. Lampman, G. A. Kriz, and J. R. Vyvyan, Introduction to Spectroscopy, 5th Edition, Brooks-Cole, 2009*
4. *G. M. Barrow, 'Introduction to Molecular Spectroscopy', McGraw Hill, 1962.*
5. *R. M. Silverstein, F. X. Webster, D.J. Kiemle, Spectroscopic identification of organic molecules, 7th Edition, John Wiley*
6. P. S. Kalsi, Spectroscopy of Organic Compounds: New Age International Pvt Ltd 6th edition edition,, 2006

REFERENCE:

1. *Hollas, J.M., Modern Spectroscopy, John Wiley & Sons, Fourth Edition, 2004*
2. *J. Keeler, Understanding NMR spectroscopy, Wiley, 2009*
3. *D. A. Skoog, F. J. Holler and S. R. Crouch, 'Principles of Instrumental Analysis', 6th Edition, Thomson Brooks/Cole, 2007.*

4. *W. Kemp, NMR in Chemistry, McMillan, 1988*
5. *J. E. Wertz and J. R. Bolton Electron Spin Resonance, Springer Science*

18CHY513 Organic Reaction Mechanism 3 1 0 4

Course Outcomes

CO1: Capacity to understand nuclephile and electrophile groups and their properties
CO2: Ability to describe and demonstrate the importance of molecular rearrangements in organic compound synthesis and understand the basics of photochemistry and pericyclic reactions
CO3: Ability to describe the interaction of excited states with their surroundings and analyse photo-induced electron transfer/excitation energy transfer reactions.

Unit 1 Nucleophilic Substitution:
SN1, SN2, and Borderline (ion pair), SNi, SET mechanisms, Neighboring group participation, substitution at allylic carbons, substitution at aliphatic trigonal carbon, substitution at vinylic carbon. Effect of substrate structure, nucleophile, leaving group and medium on reactivity. Ambident nucleophiles and substrates. Aromatic nucleophilic substitution: SNAr, SN1, benzyne and SRN1 mechanisms. Effect of substrate structure, leaving group and attacking nucleophile on reactivity.

Unit 2 Electrophilic substitution:
SE2 and SEi, SE1, substitution accompanied by double bond shift. Effect of substrate, leaving group, and solvent on reactivity. Aromatic electrophilic substitution: Arenium mechanism, Structure – reactivity relationship, substituent effect, o/p ratio, ipso substitution, orientation and reactivity, quantitative treatment.
Free radical reactions: Radical addition. Effect of substrate (aliphatic, aromatic, bridgehead), nature of the radical and solvent on reactivity.

Unit 3 Addition reactions:
Mechanism of Electrophilic, nucleophilic and radical addition. Addition to conjugated systems. Orientation and reactivity. Addition of hydrogen halides, Oxymercuration, halogenation, sulfenylation, selenylation, addition involving epoxides, addition via organoborane. Addition of water, alcohol, sulfides, to aldehydes, ketones, imines, isothiocyanates, nitrocompounds, nitriles. Mannich reaction,
Elimination reactions: Mechanism of elimination reactions E2, E1, E1CB, steric effect. Effect of substrate structure, base, leaving group and medium on reactivity. Mechanism of pyrolytic elimination.

Unit 4 Rearrangement reaction:

Mechanism of Nucleophilic, electrophilic and radical rearrangements. Nature of migration, migratory aptitudes, memory effects. Wagner-Meerwein, Pinacol, Demyanov, dienone-phenol, Benzil-Benzilic acid, Favorskii, Wolff, Neber, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger, Stevens, benzidine, Hofmann-Loffler and Chapman rearrangements and their mechanisms.

Unit 5 Photochemistry and pericyclic reactions:

General principles – Fate of excited state – Jablonsky diagram - chemical process – Photochemistry of alkenes, dienes and polyenes, Carbonyl compounds, Norrish type 1 and Type 2, Patterno –Buchi reaction.

Pericyclic reactions: Cyclo addition - Diels-Alder reaction, Substituent effect on reactivity, regioselectivity and stereochemistry, Catalysis of Lewis acids, Synthetic applications, Enantio selective Diels alder reactions, Intramolecular Diels-Alder reactions. 1,3 Dipolar Cycloaddition – reactivity, regio and stereoselectivity, Applications. [2+2] cycloaddition – ketenes and alkenes – photochemical Electrocyclic reactions, Orbital symmetry, charged species. Sigmatropic rearrangements – [1,3], [1,5], and [1,7] sigmatropic shifts – [3,3] sigmatropic rearrangements – Cope, Oxy-Cope and Claisen rearrangement. [2,3] rearrangements – oxides and ylides –Wittig and aza – Wittig rearrangements, Cheletropic reactions.

TEXT BOOKS

1. Michael B Smith, "March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure", 7th edition, Wiley (2015).
2. Francis A.Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part A: Structure and Mechanisms", 5th Edition, Springer, 2008
3. Francis A.Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part B: Reactions and Synthesis", 5th Edition, Springer, 2008.
4. Singh S P and SM Mukherji, "Reaction Mechanism in Organic Chemistry", 2014

REFERENCES

1. Reinhard Bruckner, Advanced Organic Chemistry, Reaction Mechanisms, Elsevier, 2002
2. R.O.C. Norman and J.M. Coxon, "Principles of organic synthesis", CRC press, 2014
3. Ian Fleming, Frontier Orbitals and Organic Chemical Reactions 1st Edition, Wiley, 1991

18CHY514 Heterocyclic and Natural Product chemistry 3 0 0 3

Course Outcome

CO1: able to explain on mechanistic level reactions and synthesis of important nitrogen/oxygen/Sulphur containing heterocycles; pyrroles, pyridines, diazoles, diazines, benzo-condensed analogs, furan and thiophenes
CO2: Understand the fundamentals of carbohydrate chemistry
CO3: Provide an overview of field of biochemistry and natural product chemistry, their occurrence, structure, total synthesis, biosynthesis and properties.

Unit 1 Heterocyclic compounds
Nomenclature and general characteristics of heterocyclic compounds, study of three and four-membered ring heterocyles containing one heteroatom, structure and synthesis of penicillin and cephalosporin-C, structure and synthesis of reserpine, heteroaromatic compounds (five and six-membered rings) containing one and two heteroatoms, fused ring compounds - indole, quinoline, isoquinoline, coumarin, flavones, purine and pyrimidine, bases present in nucleosides.

Unit 2 Carbohydrates and nucleic acids
Nomenclature – aldoses, ketoses, furanoses, pyranoses. Classification – monosaccharides, disaccharides and polysaccharides. Structure (Fischer, Haworth and chair projection) of ribose, glucose, fructose, maltose, sucrose, lactose, starch, cellulose and cyclodextrins. Preparation of alditols, glycosides, deoxysugars. Biosynthesis of vitamin C from glucose. Structure and synthesis of nucleic acids, genetic code, recombinant DNA. biosynthesis of shikimic acid

Unit 3 Chemistry of Natural Products
Alkaloids - classification, structure elucidation based on degradative reactions (quinine atropine), Terpenoids - classification, structure elucidation and synthesis of abietic acid, terpenoids. Total synthesis of quinine and papavarine (morphine, heroin)

Unit 4 Steroids
Steroids - classification, structure of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone, classification, structure and synthesis of prostaglandins, biosynthesis of fatty acids, prostaglandins, and steroids.

Unit 5 Amino acids, Peptides and Enzymes
Synthesis of amino acids - Strecker and azlactone synthesis, reactions of amino acids, structure of proteins, introduction to enzymes and coenzymes with special reference to the function of chymotrypsin, NAD, thiamine, pyridoxal, solid phase synthesis – choice of resin, classification and reactions leading to peptide formation.

TEXT BOOKS:

1. I.L. Finar Organic Chemistry vol 2 (3rd.ed.) Longmans Green & Co. 1964
2. Sujata V. Bhat, Bhimsen A. Nagasampagi, Meenakshi Sivakumar, Chemistry of Natural Products, Springer 2005

REFERENCES:

1.K. C. Nicolaou, Eric J. Sorensen, Classics in Total synthesis, Wiley, 1996.
2. Ashutosh kar, Chemistry of Natural Products, (Volume I and II), CBS

18CHY515 Organometallic Chemistry 3 0 0 3

Course Outcomes

CO1: Ability to describe the chemistry of metal carbonyls, their synthesis and nature of bonding.
CO2: Capability to understand the fundamentals of types of organometallic compounds, their structure, bonding.
CO3: Ability to demonstrate the stereochemistry of organometallic compounds using multinuclear magnetic resonance spectroscopy and important chemical transformation using organometallic reagents.

Unit 1: Concepts and Metal Carbonyls
History and overview on organometallic compounds. Classification and nomenclature – hapticityof fragments, 18-electron and 16-electron organometallic compounds. Structure prediction based on '18 electron rule'. Metal carbonyls – synthesisand bonding of metal carbonyls (based on MO theory), donor and acceptor properties of CO, different types of binding modes of CO, poly-nuclear carbonyls with and without bridging groups, metal-metal bonding in M-CO clusters, cluster valence electron (CVE) count, CVE based structure prediction. IR spectral features of metal carbonyls, activation of CO by bonding with metal ions.

Unit 2: Types of organometallic compounds
Metal phosphines compounds of transition metals, M-N_2 (metal dioxygen), M-O_2 (metal dioxygen), M-NO (metal nitrosyl) and M-CN (metal cyanide/isocyanide) complexes, bonding and structural features. Organometallic compounds with π-donor ligands like olefins, acetylenes and allyl moieties. Metal derivatives of cyclic π-donors (metallocenes, sandwich/half-sandwich compounds, bent metallocenes), metal-carbon σ-donors (metal carbenes – Fischer carbenes, Schrock carbenes and *N*-heterocyclic carbenes, metal polyenes, metal carbines, metal alkyl/aryl derivatives). Organometallic chemistry of lithium and magnesium, aluminum alkyls and all other main-group organometallics. Structural features and nature of bonding in above compounds.

Unit 3: Structure and Bonding
Fragment molecular orbitals (FMO) of various organic and inorganic moietieslike CH_3, CH_2, CH, BH_2, BH, NH_2, NH. FMO's (π-orbitals) of C_3H_5, C_4H_4, C_4H_6, C_5H_5, C_6H_6, C_8H_8. Inorganic

fragments MLn with varying number of L's. Symmetry and shape of their FMO's. Isolobal concept, iso-electronic and isolobal relationships between various organic and inorganic (ML_n) fragments. Structure and bonding between various organic and inorganic fragments based on MO level diagrams – metal-olefins, ML_n-cyclobutadiene, ML_n-carbene, ML_n-carbyne, ML_n-cyclopentadienyl systems, compounds with metal-metal multiple bonds (metal-metal σ, π and δ bonds).

Unit 4: Stereochemistry and reactions

Stereochemically non-rigid molecules, fluxional nature of organometallic compounds (including Li-C, Mg-C), characterization of non-rigidity of organometallic compounds by NMR spectroscopy. Difference in NMR spectra of fluxional organometallic compounds at high and low temperatures. Characterization techniques of organometallic compounds (by NMR – ^{1}H, ^{13}C and ^{31}P NMR spectroscopy, Dynamic NMR, Mass spectrometry). Reactions involving various organometallic compounds - oxidative addition reactions, reductive elimination reactions, migratory insertion reactions, 1,1-type and 1,2-type insertion reactions, elimination reactions, β-hydride elimination reactions. Conditions for organometallic compounds to exhibit above reactions, cyclo-metalation and ortho-metalation reactions, agostic interactions.

Unit 5: Organometallic Catalysis

Alkene hydrogenation using Wilkinson's catalyst, water-gas shift reaction, Mosanto process, Cativa Process. Reaction steps in the above catalytic processes. Hydro-formylation reactions, catalytic addition of molecular oxygen to alkenes (Wacker process), Ziegler-Natta polymerization of alkenes, Fischer-Tropsch process, olefin-metathesis (types of Grubbs catalysts and Hoveyda–Grubbs catalysts), oligomerization of alkynes, aluminum alkyls in polymerization of olefins. Palladium based reactions such as Heck, Stille, Suzuki, Sonogashira, Buchwald-Hartwig couplings; Tsuji-Trost C-C bond formations. Homogeneous vs. heterogeneous organometallic catalysis (principles, mechanism and their applications). Organometallics - in industry, in medicine, in agriculture and in environmental science.

TEXTBOOKS:

1. J.E. Huheey, R.A. Keiter, R.L. Keiter, 'Inorganic Chemistry-Principles of Structure and Reactivity', 4thEdn., Prentice Hall, 1997.
2. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong,' Shriver and Atkins Inorganic Chemistry', 4thEdn., Oxford University Press, 2006.
3. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, 'Advanced Inorganic Chemistry', 6thEdn.,Wiley-Interscience, 1999.
4. Anil Elias, Gupta B.D., "Basic Organometallic Chemistry", Universities Press; 2ndEdition 2013
5. J.D. Atwood, 'Inorganic and Organometallic Reaction Mechanism', 2nd Edn., Wiley-

REFERENCES:

1. R. H. Crabtree, 'Organometallic Chemistry of the Transition Metals', John Wiley & Sons, 6th Ed.
2. VCH, 1997.

3. J. Tsuji, 'Transition metal reagents and catalyst innovations in organic synthesis', John-Wiley- & Sons, Ltd, New York, 2000
4. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rdEdn., Wiley-India, 2007.
5. M. Bochmann, Orgaonometallics: Complexes with Transition Metal-Carbon Sigma Bonds, Oxford University Press, 1994.
6. J. P. Collman, R G Finke and and J R Norton "Principles and Applications of Organo-transition metal Chemistry" University Science Books, 1987.
7. W.K. Li, G.D. Zhou, T. Mak, Advanced Structural Inorganic Chemistry, Oxford University Press, 2008.

K. C. Nicolaou, 'Classics in Total Synthesis', Vols I-III, Wiley-VCH, 1996; 2003; 2011

18CHY583 ADVANCED PHYSICAL CHEMISTRY LAB 0 0 5 2

Course Outcomes

CO1: Development of skill to evaluate the kinetics of different chemical reactions and to determine the activation energy for reactions.
CO2: Ability to analyse the thermodynamic parameters in phase equilibrium
CO3: Learn the optical properties of materials and apply this for analytical applications
CO4**:** Acquire knowledge to create experiments to evaluate physical chemistry concepts.

Experiments:

1. Construction of phase diagram for three component system.
2. Determination of equivalent conductance at infinite dilution of weak electrolytes.
3. Determination of order of reaction for ion exchange reaction.
4. Extraction efficiency of solute from a solution by immiscible solvent method.
5. Determination of calorific value using Bomb calorimeter.
6. Kinematic viscosity of lubricants using Bomb calorimeter.
7. Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometerically.
8. Determination of flash point, fire point of a lubricant.
9. Determination of cloud point and pour point of a lubricant.

TEXTBOOKS:

1. *Alexander Findly, 'Practical physical chemistry', 9th edition, Wiley, 1972.*
2. *R.C.Das and B.Behera, 'Experimental Physical Chemistry', Tata McGraw-Hill, 1983.*

REFERENCE BOOKS:

1. *J.B.Yadav, 'Advanced Practical Physical Chemistry', Krishna Prakashan Media, 29th edition, 2010.*
2. *Francis William Gray, 'A Manual of Practical Physical Chemistry' Macmillan and Co., Limited, 1914.*

18CHY584 INORGANIC QUANTITATIVE ANALYSIS LAB 0 0 6 2

Course Outcomes

CO1: Development of skill to perform classical quantitative analysis of metals in a mixture of inorganic compounds
CO2: Development of adequate knowledge of the chemistry involved in the estimations of various compounds in commercial samples.
CO3: Attainment of knowledge and skill in activities related with effective and safe functioning of a chemistry lab.

1. Estimation of Calcium (Permanganometry)
2. Estimation of Barium (Iodometry)
3. Estimation of Calcium as Calcium Carbonate (Gravimetry)
4. Estimation of Zinc using oxine (Gravimetry)
5. Estimation of Iron as Ferric Oxide (Gravimetry)
6. Analysis of Brass
7. Estimation of Copper and Nickel in a Mixture
8. Estimation of Copper and Iron in a Mixture
9. Preparation and Determination of Ferrous Oxalate
10. Estimation of Different Types of Hardness in the Given Water Sample
11. Estimation of Different Types of Alkalinities in the Given Water Sample
12. Estimation of Dissolved Oxygen in the Given Water Sample
13. Complexometric Estimations

TEXTBOOKS:

1. G. Svehla, 'Vogel's Qualitative Inorganic Analysis', 7th Edition', Prentice Hall, 1996.
2. D.A.Skoog and D.M.West ,'Analytical Chemistry - An Introduction', 4th Edition, CBS Publishing Japan Ltd., 1986.

REFERENCES

1. E.J.Meehan, S.Bruckenstein and I.M.Kolthoff and E.B.Sandell, 'Quantitative Chemical Analysis', 4th Edition, The Macmillan Company, 1969.

2. R.A.Day (Jr) and A.L.Underwood, 'Quantitative Analysis', 6th Edition, Prentice Hall of India, 1991.

18AVP501 AMRITA VALUES PROGRAMME 1 0 0 1

Amrita University's Amrita Values Programme (AVP) is a new initiative to give exposure to students about richness and beauty of Indian way of life. India is a country where history, culture, art, aesthetics, cuisine and nature exhibit more diversity than nearly anywhere else in the world.

Amrita Values Programmes emphasize on making students familiar with the rich tapestry of Indian life, culture, arts, science and heritage which has historically drawn people from all over the world.
Post-graduate students shall have to register for any one of the following courses, in the second semester, which may be offered by the respective school.

Courses offered under the framework of Amrita Values Programme: **Art of Living through Amma**

Amma's messages can be put to action in our life through pragmatism and attuning of our thought process in a positive and creative manner. Every single word Amma speaks and the guidance received in on matters which we consider as trivial are rich in content and touches the very inner being of our personality. Life gets enriched by Amma's guidance and She teaches us the art of exemplary life skills where we become witness to all the happenings around us still keeping the balance of the mind.

Insights from the Ramayana

Historical significance of Ramayana, the first Epic in the world – Influence of Ramayana on Indian values and culture – Storyline of Ramayana – Study of leading characters in Ramayana – Influence of Ramayana outside India – Misinterpretation of Ramayana by Colonial powers and its impact on Indian life - Relevance of Ramayana for modern times.

Insights from the Mahabharata

Historical significance of Mahabharata, the largest Epic in the world – Influence of Mahabharata on Indian values and culture – Storyline of Mahabharata – Study of leading characters in Mahabharata – Kurukshetra War and its significance – Importance of Dharma in society – Message of the Bhagavad Gita - Relevance of Mahabharata for modern times.

Insights from the Upanishads

Introduction: Sruti versus Smrti - Overview of the four Vedas and the ten Principal

Upanishads - The central problems of the Upanishads – Ultimate reality – thenature of Atman - the different modes of consciousness - Sanatana Dharma and its uniqueness - The Upanishads and Indian Culture – Relevance of Upanishads for modern times – A few Upanishad Personalities: Nachiketas, SatyakamaJabala, Aruni, Shvetaketu.

Insights from Bhagavad Gita

Introduction to Bhagavad Gita – Brief storyline of Mahabharata - Context of Kurukshetra War – The anguish of Arjuna – Counsel by Sri. Krishna – Key teachings of the Bhagavad Gita – Karma Yoga, Jnana Yoga and Bhakti Yoga - Theory of Karma and Reincarnation – Concept of Dharma – Idea of the Self and Realisation of the Self – Qualities of a Realised person - Concept of Avatar - Relevance of Mahabharata for modern times.

Swami Vivekananda and his Message

Brief Sketch of Swami Vivekananda's Life – Meeting with Guru – Disciplining of Narendra - Travel across India - Inspiring Life incidents – Address at the Parliament of Religions – Travel in United States and Europe – Return and reception India – Message to Indians about our duties to the nation.

Great Spiritual Teachers of India

Sri Rama, Sri Krishna, Sri Buddha, AdiShankaracharya, Sri Ramanujacharya, Sri Madhvacharya, Sri Ramakrishna Paramahamsa, Swami Vivekananda, Sri Ramana Maharshi, Mata Amritanandamayi Devi

Indian Arts and Literature:

The aim of this course is to present the rich literature and culture of Ancient India and help students appreciate their deep influence on Indian Life - Vedic culture, primary source of Indian Culture – Brief introduction and appreciation of a few of the art forms of India - Arts, Music, Dance, Theatre, Paintings, Sculpture and architecture – the wonder language, Sanskrit and ancient Indian Literature

Importance of Yoga and Meditation in Life:

The objective of the course is to provide practical training in YOGA ASANAS with a sound theoretical base and theory classes on selected verses of Patanjali's Yoga Sutra and Ashtanga Yoga. The coverage also includes the effect of yoga on integrated personality development.

Appreciation of Kerala's Mural Art Forms:

A mural is any piece of artwork painted or applied directly on a wall, ceiling or other large permanent surface. In the contemporary scenario Mural painting is not restricted to the permanent structures and are being done even on canvas. A distinguishing characteristic of mural painting is that the architectural elements of the given space are harmoniously incorporated into

the picture. Kerala mural paintings are the frescos depicting mythology and legends, which are drawn on the walls of temples and churches in South India, principally in Kerala. Ancient temples, churches and places in Kerala, South India, display an abounding tradition of mural paintings mostly dating back between the 9th to 12th centuries CE when this form of art enjoyed Royal patronage. Learning Mural painting through the theory and practice workshop is the objective of this course.

Practicing Organic Farming

Life and nature are closely linked through the healthy practices of society for maintaining sustainability. When modern technological knowhow on microorganisms is applied in farming using the traditional practices we can avoid damage to the environment. The course will train the youth on modern practices of organic farming. Amma says "we have to return this land to the coming generations without allowing even the slightest damage to happen to it". Putting this philosophy to practice will bring about an awakening and enthusiasm in all to strive for good health and to restore the harmony in nature"

Ancient Indian Science and Technology

Science and technology in ancient and medieval India covered all the major branches of human knowledge and activities, including mathematics, astronomy, physics, chemistry, medical science and surgery, fine arts, mechanical, civil engineering, architecture, shipbuilding and navigation. Ancient India was a land of sages, saints and seers as well as a land of scholars and scientists. The course gives an awareness on India's contribution to science and technology.

Course Outcomes:
CO1: Understanding Indian Value system
CO2: Learning for Indian historical epics
CO3: Understandin the importance of Yoga ,Meditation in Life and organic farming.

18CHY601 ELECTROCHEMISTRY, ENERGY, SYSTEMS AND KINETICS 3 1 0 4

Course Outcomes

CO1: Attainment of sound theoretical knowledge in the science, applications and characterization of surfaces and colloidal state.
CO2: Development of sound theoretical and analytical knowledge in electrochemical principles (both in ionics and electrodics)
CO3: Ability to apply the electrochemical principles for solving problems and fabrication of energy storage devices and electrolysis processes.
CO4: Development of analytical skills to predict the speed of chemical reactions and the conditions for reactions with high yield.
CO5**:** Sound theoretical knowledge in catalysis and photochemical reactions and exploring its applications in improving the product yield.

Unit 1 Surface Chemistry
Different types of interfaces, molecular and atomic surface structure, surface chemical reactions, surface tension of solutions, surface excess, thermodynamics of surfaces, Gibbs equation and its derivation, surface films, surface potential, adsorption by solids, Langmuir isotherm - its kinetic and statistical derivation, Freundlich equation, multilayer adsorption, BET isotherm - its kinetic derivation, measurement of surface area, colloids - their preparation, purification, stability & electro kinetic phenomena, Donnan membrane equilibrium, micro and nano emulsions, surface analysis using photoelectron spectroscopy, surface imaging techniques like SEM, TEM, AFM etc., sputter coating, ion beam principles, design of surfaces with novel properties.

Unit 2 Electrochemistry I
Faraday's law, conductivity of electrolytes, applications of conductivity measurements, ionic mobility, transference number, Debye-Huckel-Onsagar equation of conductivity and its validity for aqueous and nonaqueous solutions, deviations from the Onsagar equation, activity and activity coefficients in electrolytic solution, Debye-Huckel theory and its tests and improvements, Onsager equation, electrochemical potential, electric potential at interfaces,

Unit 3 (a) Electrochemistry II
Electrochemical cells, standard electrode potentials, reversible cell, concentration cells with and without transference, energetic of cell reactions, effect of ionic concentration, pressure and temperature on the energetic of cell reactions, applications of e.m.f. measurements, potentiometric measurement of pH, glass electrode and its structure, performance and limitations, double layer, charge transfer across interfaces, polarisation, concentration polarisation, decomposition potential, over potential (hydrogen, oxygen and metal decomposition over voltage), theories of over voltage, electrode kinetics - Butler Volnmer equation, Tafel equation, power generation, storage cells, theories of corrosion, fuel cells, diffusion potential, liquid junction potential, Henderson's equation, electron transfer kinetics - Marcus theory, electrochemical impedance spectroscopy, electro organic chemistry - electro
oxidation, electro reduction, electro polymerisation.

Unit 3 (b) **Batteries and Fuel Cells**
Primary, secondary and reserve batteries, chemistry, fabrication, performance aspects, packing classification and rating of Zn-C, Mg, alkaline manganous dioxide, mercuric oxide, silver oxide batteries, Zn/air and Li button cells, solid electrolyte cells, secondary batteries - lead-acid, Ni-Cd, Ni-Zn, Li and Li+ batteries, rechargeable Zn-alkaline batteries, reserve batteries – zinc-silver oxide, lithium anode cell, thermal batteries, advanced batteries for electric vehicles – metal/air, Zn-Br, sodium-beta and lithium/iron sulpfide batteries, Fuel Cells – carbon, hydrogenoxygen, methanol, molten carbonate, solid polymer electrolyte and biochemical fuel cells, alkaline fuel cells, phosphoric acid fuel cells, solid oxide fuel cells, proton exchange membrane fuel cells, solar cells – photovoltaic and photo electrochemical
cells, photo biochemical conversion cell

Unit 4 Chemical Kinetics I

Reaction rates and order of reactions, determination of order of reactions, complex reactions, reversible, consecutive and concurrent reactions, reactions of variable order, steady state treatment, reaction mechanism and molecularity, theories of unimolecular reactions and termolecular reactions, Arrhenius equation, collision theory and transition state theory, comparative study of the theories of reaction rates, free energy of activation, effect of solvent on rate of reactions, ionic reactions and effect of ionic strength - salt effect, effect of pressure on velocity of gas reactions.

Unit 5 Chemical Kinetics II

Reaction dynamics, fast reactions, flash photolysis and relaxation methods, catalysis and inhibition, homogeneous catalysis, acid, base and enzyme catalysis, kinetics of enzyme catalyzed reaction - the Michaelis-Menten equation, photochemical kinetics, steady state treatment of photochemical reactions, Semenov-Hinshelwood theory of chain reactions and explosions, free radical reactions - the Rice-Herzfeld mechanism.

TEXTBOOKS:

1. *K. J. Laiddler, 'Chemical-Kinetics', 3rd Edition, McGraw Hill, New York, 2004.*
2. *Dell, Ronald M Rand and A.J David, 'Understanding Batteries', 1st edition, Royal Society of Chemistry, 2001.*

REFERENCES:

1. *M. Aulice Scibioh and B. Viswanathan, 'Fuel Cells-Principles and Applications', reprint,*
1. *University Press, India, 2006.*
2. *Gilbert W. Castellan, "Physical Chemistry", 3rd Edition, Narosa Publishing House, 2004.*
3. *Lindon David, 'Handbook of Batteries', 3rd edition, McGraw Hill, 2002.*
4. *W. J. Moore and R. G. Pearson, 'Kinetics and Mechanism', 2nd edition, Wiley, 1981.*

18CHY602 Synthetic Strategies and Reagents 3 1 0 4

Course Outcomes

CO1: Understand the principles, concept and application of reterosynthesis

CO2: Utilise organometallic chemistry and protecting group strategy in planning the synthesis of complex target compounds.

CO3: Understand the functional group interconversions and the formation of carbon-carbon, C-N, C-O bonds by using various reagents and protecting groups.

CO4**:** Appreciate the role of the synthetic organic chemist in pharmaceutical and agricultural research and development.

Unit 1 Synthetic Strategies

Synthetic strategies: Functional group inter-conversion – conversion of one functional group to other. Nitrogen, oxygen, sulphur protection and deprotection – utilization of protection groups in organic synthesis. Retro synthetic analysis, functional group equivalents, use of retrosynthesis in organic synthesis. Reversal of reactivity (Umpolung), Introduction to combinatorial chemistry. Application of phase transfer catalysts.

Unit 2 Oxidation and reduction:

PCC, DDQ, DMSO, Dess-Martin Reagent, TEMPO, osmium tetroxide, ruthenium tetroxide, selenium dioxide, peracids, hydrogen peroxide, singlet oxygen, aluminum isopropoxide, periodic acid, lead tetraacetate. Swern, Jones, Oppeneur oxidation, Woodward and Prevost hydroxylation, Sharpless asymmetric epoxidation, catalytic hydrogenations (heterogeneous and homogeneous), Clemmenson, Wolff Kishner, Rosenmund and MPV reductions, metal hydrides as reagents (aluminium/boron hydrides and hydroboration reaction), Birch reduction, Borche Reduction, hydrazine and diimide reduction.

Unit 3 Organometallic reagents: Preparation, properties and reactions of organo lithium, organosilicon, organozinc (Reformatsky reaction) and organomagnesium reagents (Barbier and Grignard), organocadmium, organo mercury reagents based organometallic reactions involving C-C bond formation. Selected functional group transformations in organic synthesis. Preparation and reactions of Organo copper, organopalladium,- Wacker process – Heck reaction, cross coupling, carbonylation reaction, organonickel, organo cobalt and organo rhodium reagents – Olefin metathesis reaction. Reactions and applications of Organoboron, organo silicon and organotin compounds.

Unit 4 C-C, bond formation

C-C bond formation – aldol, Arndt-Eistert, Bardhan-Sengupta, Baker-Venkataraman, Barbier, Baylis-Hillman, Benzoin, Heck, Fukuyama, Dieckmann, Friedel–Crafts, Michael, Perkin, Claisen, Robinson annulations, Vilsmeier, Wittig, Knoevnagel, Michael additions.

Unit 5 C-N, C-O bond formations

C-O bond formation – barton, Fischer esterification, Prins, Darzen, Baeyer-Villiger, Mitsunobu, Williamson's ether synthesis, Ullman Coupling with Boronic Acids.

C-N bond formation – Mannich, Fukuyama, Mitsunobu, Ritter, Gabriel Synthesis, Ugi, Doebner Reaction, Buchwald-Hartwig, Stork-enamine, formation of azides and hydrazines, formation of amides and peptides, coupling reactions.

TEXT BOOKS

1. Modern Organic Synthesis, Dale L. Boger, The Scripps Research Institute, Rush Press, San Diego, California, 2001
2. Francis A.Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part B: Reactions and Synthesis", 5th Edition, Springer, 2008.
3. R.O.C. Norman and J.M. Coxon, "Principles of organic synthesis", CRC press, 2014

REFERENCES

1. Stuart Waren, Designing Organic Synthesis: A programmed introduction to the synthon approach, JOHN WILEY & SONS, 2nd edition, 2008
2. Name Reactions: A collection of detailed Mechanisms and synthetic applications, Jie Jack Li, Springer, fourth edition (expanded edition), 2009.
3. Michael B Smith, "March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure", 7th edition, Wiley (2015).
4. Francis A.Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part A: Structure and Mechanisms", 5th Edition, Springer, 2008

18CHY603 Solid State Chemistry and Materials Science 3 0 0 3

Course Outcomes

CO1: Ability to understand the various modes of arrangement of atoms in a crystal system
CO2: Apply basic rules of **electron orbitals** to predict molecular structure and properties
CO3: Understand the various methods involved in the synthesis of solid state materials
CO4: Apply various analytical techniques for the characterization of solid state materials.

Unit 1 Introduction to Crystal Systems

Introduction to solids - solid state chemistry, close packing, hcp, fcc, density, coordination numbers, tetrahedral and octahedral holes, body centered and primitive structures, symmetry, proper rotation, mirror planes, inversion, improper axis symmetry elements, symmetry in crystals, Schoenflies and Hermann-Mauguin notations, unit cells, glide plane, screw axis, atom occupancy in cubic unit cells, seven crystal systems/classes, space groups, Miller indices, Bravais lattices, reciprocal lattice, inter-planar spacing in different crystal systems, fractional coordinates, ionic solids, structures of CsCl, NaCl, NiAs, zinc blende and wutzite structures, MX_2 type solids, fluorite and antfluorite structures, $CdCl_2$ and CdI_2 structures, rutile and anti-rutile, ReO_3, spinel and inverse spinel, pervoskite structures, ionic radii, crystal radii, radius ratio, Extended covalent array, diamond, graphite.

Unit 2 Bonding in Solids and Electronic properties

Bonding in crystals, metallic bonding, ionic bonding, covalent bonding, silicates, Born-Haber cycle, Hess's law, lattice energy (L) and calculation of L, free electron theory, density of states, electronic conductivity, molecular orbital theory, overlap and bonding, linear chain of H atoms, LCAO, Fermi Level, conductors, insulators and semiconductors, n- and p-type semiconductors, bands in compounds, band-gap energy, direct and indirect band gaps in semiconductors, band-gap measurements, electrical conductivity, photo-conductivity.

Unit 3 Magnetic and Optical Properties of Solids

Behaviour of substances in magnetic field, magnetic moments, para magnetism, diamagnetism, ferro- and anti-ferromagnetism, ferri-magnetism, effects of temperature of magnetism, Curie & Curie-Weiss laws; mechanism of ferro- and anti-ferromagnetic ordering, super exchange. Luminescence and phosphorescence of solid materials, phosphors, lasers, non-stoichiometry and its effect in properties of solids, electronic properties of non-stoichiometric oxides. Defects in solids, Schottky defects, Frenkel defects, doping in crystals and colour features, ruby, diamond, organic conductors, preparation, mechanism of conduction in organic semiconductors, photoconductivity of polymers.

Unit 4 Materials Science-Structure and properties

Solid materials of importance. Structure and properties of SiO_2, ZrO_2, SiC, BN, ZnO, TiO_2, CdS, CdTe, GaAs, MoS_2. Band-gap properties of semiconductors like ZnO, TiO_2, CdS, CdSe, CdTe, GaAs, MoS_2 and $(CH_3NH_3)[PbX_3]$-type perovskites. Photo-catalytic properties of ZnO and TiO_2 – principle and applications. Inorganic-organic hybrid materials. High Tc superconductors (HTS) like Bi-Sr-Ca-Cu oxide based HTS (BSCCO) and Y-Ba-Cu-oxide (YBCO), their structure and properties. Metal-organic framework (MOF) materials, special features of MOF materials. Synthesis, special features and properties of MOF materials like HKUST-1 and MOF-8. Gas storage and emission properties of MOF materials. MOFs as sensors. Zeolites, their special features and properties.

Unit 5 Materials Science-Synthesis, processing and characterization

Sol and gel, their properties, xerogels. Sol-gel synthesis - synthesis of SiO_2 and TiO_2 through sol-gel process. Calcination and sintering. Characterization of processed materials, PXRD, IR, Raman, Uv-visible and solid state NMR spectral techniques. Understanding morphological features through, SEM, EDAX and TEM methods. Chemical vapour deposition (CVD) method. Solid state synthesis, synthesis of High Tc superconducting materials like YBCO and BSCCO. Synthesis of inorganic-organic hybrid materials. Solvo-thermal and high pressure synthesis.

TEXTBOOKS:

1. *L V Azroff , 'Introduction to Solids' , Tata McGraw-Hill publishing company*
2. L. E. Smart and E. A. Moore, Solid State Chemistry – An Introduction, 4th Edition, CRC Press, 2016.
3. A. R. West, Solid State Chemistry and its Applications, Wiley, 2014
4. C N R Rao, K Biswas, Essentials of Inorganic Materials Synthesis, John Wiley, 2014
5. C N R Rao Chemical Approaches to Synthesis of Materials, Wiley, 1994

REFERENCES

1. D. Jiles, "Magnetism and Magnetic Materials", Chapman and Hall, London, 1991.
2. R. E. Hummel, "Electronic Properties of Materials", 3rd ed., Springer-Verlag, New York, 2001.
3. Schubert, U. and Hüsing, N, Synthesis of Inorganic Materials, 3rd edn, VCH-Wiley Verlag GmbH, Weinheim, 2012

4. W.D. Kingery, H.K. Dowen and R.D. Uhlman, Introduction to Ceramics, John Wiley.
5. F.H. Norton, Elements of Ceramics,.
6. M.W. Barsoum, Fundamentals of Ceramics, McGraw Hill.
7. Material Science and Engineering, S.K. Hajra Choudhury, Indian Book Dist.
8. B D Fahlman, Materials Chemistry, 2nd Edition, Springer, 2011
9. Stefan Kaskel, The Chemistry of Metal–Organic Frameworks: Synthesis, Characterization, and Applications, Wiley-VCH Verlag GmbH, 2016

18CHY604 Bio-inorganic Chemistry 3 0 0 3

Course Outcomes:

CO1 Skill to apply the principles of coordination chemistry in understanding functions of biological systems.
CO2 Sound knowledge in the interaction of metal ions with biological environments.
CO3 Able to explain how the nature adapts certain properties of metal centres for specific applications and the role of metal ions in metalloenzymes for catalysing reactions that are energetically and stereo selectively very difficult.
CO4 Skill in understanding the mechanism of metalloenzymes by applying the suitable spectroscopic and other techniques
CO5 Understanding the role of metal ions as diagnostic and therapeutic agent. Also have the ability to explain the mechanism of metal toxicity.

Unit 1:
Basics in bio-inorganic chemistry
Essential elements in biological systems, transport of ions across biological membranes, active and passive transport, metal transport and metallochaperons, Na+/K+ pump and active transport. Metal complexation with biological molecules. Electron transport in biology, electron transport chain (ETC), role of ETC in biological systems. Amino acids, peptides and proteins, primary and secondary structure of proteins, α-helix and β-sheets forms of proteins and their special features; tertiary and quaternary structures of proteins the type of molecular interactions involved in them. Reactive oxygen species (ROS), generation and function of organic free radicals, action of ROS in biological systems, oxidative stress, antioxidants. Photosynthesis, PS-I and PS–II.

Unit 2:
Oxygen take-up, transport and storage proteins
Porphine, corrin, corrole, chlorin and bacteriochlorin. Myoglobin (Mb) and hemoglobin (Hb), their prosthetic groups and functions, mechanism for reversible binding of O2 in Mb and Hb. Cooperative effect in Hb and its consequence. Behaviour of bound O2 to Fe(II). Difference between O2 and CO binding to Hb and Mb, CN– poisoning. Structure and functions of haemerythrin (Hr) and haemocyanin (Hc), O2 binding nature in Hr and Hc, electron transfer processes in them. Cytochromes and their role in biology, cytochrome P-450, cytochrome Coxidase and oxygen transfer from O2 to non-activated substrates, monooxygenases, methane monooxygenase (MMO). Fe-S and other non-heme iron proteins, ferredoxins-their structure and special properties, transferrin, ferritin, siderophores, enterobactin, uptake, transport and storage of iron. Sickle-cell anemia

Unit 3:

Metallo-enzymes

Catalases – structure and properties reaction mechanism. Peroxidases- glutathione peroxidase, HRP, structure and properties and enzyme reaction mechanism. Cytochrome c peroxidase and lignin peroxidase. Copper enzymes-structure and function, azurin, plastocyanin. Type I, II and III copper proteins. Superoxide dismutase (SOD) - structure and enzymatic reaction mechanisms. Tyrosinase, reaction mechanism. Zn-containing enzymes, carbonic anhydrase and carboxy-peptidases-structure and enzymatic reactions. N2 fixation, nitrogenase enzyme, Fe-S clusters, Fe-protein structure, Mo-Fe protein structure, P-cluster and M-centre, their model compounds.

Unit 4:

Other functional roles of metal ions

Zn in biological systems, Zn-finger proteins – structural features and properties, classifications and their roles in biological systems. Ca2+ binding proteins, calmodulins. Metal ion based (Pt, V, Au) drugs, anticancer agents. Cis-platin and its properties. Chelation therapy, macrocyclic antibiotics. Role of Mn, Ni, Mo and Cr in biological systems, metal toxicity and homeostasis, therapeutic complexes. Diseases caused by both excess and deficiency of metal ions, thalassaemia, Wilson disease. DNA intercalators, diagnostic agents, MRI imaging and contrast agents, the role of Gd3+ and other metal ions as contrast agents.

Unit 5:

Biomimetic compounds, metals in medicine

Porphyrins (H2P) and metalloporphyrins (MP), spectral, fluorescence and redox properties of H2P and MP. Biomimetic compounds. Fe(II), Co(II) and Cu(II) based model compounds model compounds of Mb and Hc –. 'picket-fence' porphyrin and its special features. Photodynamic therapy (PDT), principles and applications. Natural and synthetic ionophores, crown ethers, interaction and uptake of alkali metal and alkaline earth metal ions with crown ethers, cryptands and cryptates, calixarenes and their special properties, cyclo-dextrins and their special properties.

TEXTBOOKS:

1. J.E. Huheey, R.A. Keiter, R.L. Keiter, Inorganic Chemistry-Principles of Structure and Reactivity, 4th Edn., Prentice Hall, 1997.
2. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley-Interscience, 1999.
3. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Shriver and Atkins Inorganic Chemistry, 4th Edn., Oxford University Press, 2006.

REFERENCES

1. S. J. Lippard, J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, 1994.
2. J. D. Atwood, Inorganic and Organometallic Reaction Mechanism, 2nd Edn., Wiley-VCH, 1997.
3. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
4. W. Kaim, B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, 1994.
5. M. N. Hughes, The Inorganic Chemistry in Biological Processes, Wiley (1981).

18CHY681 Organic Qualitative Analysis Lab 0 0 6 2

Course Outcomes:

CO1: Ability to engage in safe laboratory practices handling laboratory glassware, equipments, and chemical reagents
CO2: Capacity in predicting the outcome of some simple organic reactions, using a basic understanding of the relative reactivity of functional groups.

1. Separation of binary mixtures
Includes separation, preliminary investigations, determinations of saturation/ unsaturation, detection of elements by Lassaigne's test, functional group identification, derivative preparation, determination of melting points of the derivatives and calculation of Rf values from TLC The following mixtures can be given: (a) Acid and hydrocarbon (b) Phenol and Aldehyde (c) Phenol and acid (d) Phenol and amine (e) Acid and ester (f) Halo compound and aldehyde (g) Acid and Aldehyde (h) Amine and aldehyde (i) Amine and ketone (j) Alcohol and hydrocarbon

2. Thin layer chromatography to determine Rf values of compounds
(a) 2-nitroaniline (b) 4-nitroaniline (c) Cinnamic acid and 2-nitroaniline (d) Acetophenone (e) Ethyl benzoate 3. Simple column chromatography to separate the components of binary mixtures (a) Hydrocarbon and ester (b) Aldehyde and amine

REFERENCES:

1. P.W.G. Smith, A.J.Hannaford, B.S.Furnis and A.R. Tatchell, "Vogel's Textbook of Practical Organic Chemistry", ELBS/Longman, 1989.
2. Ralph L.Shriner, Christine K.F.Hermann, Terence C.Morrill, David Y.Curtin, Reynold C.Fuson, 'Systematic Identification of Organic Compounds', John Wiley & Sons, 2003.
3. Mann and Saunders, 'Practical Organic Chemistry', Pearson edition, 2009

18CHY682 INSTRUMENTAL AND ANALYTICAL METHODS LAB 0 0 5 2

Course Outcomes:

CO1: Development of skill to analyze the effect of electrochemical parameters for industrial anodisation.
CO2: Acquire the knowledge to apply the principles of electrolyte conductance and electrode potential for analytical applications.
CO3: Attain the skill to evaluate the optical properties of chemical species for analytical applications.

CO4: Understand the rate of electrochemical reactions and applying it for industrial corrosion.

1. Determination of strengths of halides in a mixture potentiometrically**.**
2. To find the redox potential of the given sample using cyclic voltametry.
3. Determination of half wave potential of Cd & Zn by polarography.
4. Determination of pKa of an indicator in aqueous and micellar medium using UV-Vis spectroscopy.
5. Determination of stoichiometry and stability constant of inorganic (ferric-salicylic acid) and organic (amineiodine) complexes using UV–Vis spectroscopy.
6. Determination of copper and cadmium in a mixture by electrogravimetry.
7. Determination of rate constant for enzyme kinetics-inversion of sucrose.
8. Determination of molecular weight of a polymer by Viscometry.
9. Determination of a molecular weight of a solute using Beckmann thermometer.
10. Refractrometric determination of composition of solutions.

TEXTBOOKS:

1. *Alexander Findly, 'Practical physical chemistry', 9th edition, Wiley, 1972.*
2. *R.C. Das and B.Behera, 'Experimental Physical Chemistry', Tata McGraw-Hill, 1983.*

REFERENCE BOOKS:

1. *J.B.Yadav, 'Advanced Practical Physical Chemisty', Krishna Prakashan Media, 29th edition, 2010.*
2. *Francis William Gray, 'A Manual of Practical Physical Chemistry' Macmillan and Co., Limited, 1914.*

18CHY696 Dissertation Cr 14

Course Outcomes

CO1: Capacity to demonstrate the chemical experiments related to chemical industries in the field of research and development, production unit.

CO2: Ability to analyze the structural features of chemical compound and their properties and to apply in quality control area

Employability: An ability to conduct appropriate experimentations, analyse, interpret data and apply scientific judgements to draw conclusions. Finally this work should lead to good quality publication.

ELECTIVES

18CHY633 CHEMISTRY OF BIOMOLECULES 3 0 0 3

Course Outcomes

CO1: Understand the role of aminoacids, proteins and peptides in biology along with their application.
CO2: Able to describe the basic properties, mechanisms of action and applications of enzymes
CO3: Gain knowledge in nucleic acids, antibodies, recombtinant DNAand gene analyses.

Skill: At the end of the course the student will acquire knowledge on various biomolecules and their application

Unit 1 Amino acids, Proteins and Peptides
Classification, Stereochemical aspects, physical properties, Ionic properties, spectral properties, essential and non essential amino acids, chemical reactions of amino acids, Industrial preparation and chemical synthesis of amino acids. Ionic properties of proteins, protein structure, protein purification, protein structure determination, proteomics and protein function, solid phase peptide synthesis, biologically important peptides.

Unit 2 Enzymes Introduction to Enzymes, Classification of enzymes, mechanism of enzyme action, immobilized enzymes and enzyme technology, enzyme analog built polymers, design of molecular clefts, enzymes in synthetic organic chemistry. Enzymes in biological systems

Unit 3 Molecular biology and bioinformatics
Structure of nucleic acids, genes and genome complexity, functions of nucleic acids, isolation and separation of nucleic acids, molecular analysis of nucleic acid sequences, nucleotide sequencing of DNA.

Unit 4 Immunochemical techniques
Production of antibpodies, purification and fragmentation of immunoglobulins, immunoprecipitatipon, labeling antibodies, immunoblotting, immunoassays, immunohisto/cytochemistry.

Unit 5 Recombinant DNA and genetic analysis
Constructing gene libraries, cloning vectors, hybridization and gene probes, application of gene cloning, expression of foreign genes, pharmacogenomics.

REFERENCES:

1. *Hermann Dugas, 'Bioorganic Chemistry - A Chemical Approach to Enzyme Action', 3rd edition, Springer.*
2. *Keith Wilson and John Walker, 'Principles and Techniques of Biochemistry and Molecular Biology', 6th edition, Cambridge University Press.*

18CHY634 INDUSTRIAL CHEMISTRY 3 0 0 3

Course Outcomes

CO1: To gain knowledge about various water treatment processes adopted in industries

CO2: To provide in-depth overview on production, refining and processing of various types of fuels
CO3: To understand the importance and preparative methods of explosives and chemical weapons
CO4: To learn the manufacturing process of paints and pigments and to develop ability to scale up the products prepared in the laboratory to the industrial level
CO5: To obtain a comprehensive knowledge of various energy resources used commercially
CO6: To calculate, analyse and execute different types of industrial processes

Employability: Exposure to the practices adopted in the industries aid in fetching employment in the industries involving paint manufacturing, petroleum refining and water treatment processes.
Entrepreneurship: Deep knowledge acquired on the manufacturing methods of various commercial products with insights into industrial processes helps in creating entrepreneurs.

Unit 1 Water treatment

Softening of water, Ion exchange process, Lime soda process, Modified Lime soda process, Zeolite process, Chemical and physical method of sterilization, Desalination, Boiler problems. Corrosion of boiler units, industrial water treatment, water analysis.

Unit 2 Fuels

Calorific value, determination of Calorific value, classification of fuels, Solid fuels, Properties of fuels, classification of coal, coking and non-coking coals, advantages and disadvantages of solid fuels. Liquid fuels, gaseous fuels, analysis of fuel gases, Distillation of petroleum. Processing & purification of petroleum and petroleum products, Flash point, Fire point, Knocking, antiknocking, Cetane number, octane number, natural gasoline, cracking, polymerization, alkylation, isomerisation, rocket fuels, fossil fuel, nuclear fuels.

Unit 3 Energy resources

Renewable and non renewable sources of energy, conventional and non conventional sources of energy, solar energy, solar technology, solar photovoltaic cell - application, PV lantern system, Radiotelephone system, Application of solar energy, Environmental implication, Nuclear energy, nuclear fuel cycle in India, Energy conservation and waste heat boilers, Fuel cells, hydrogen cells.

Unit 4 Paints and Pigments

White pigment, blue, green, yellow, black and red pigments - manufacture, physical properties, characteristics, Manufacture of paints, setting of paints, requirement for good paints, emulsion paint, latex paint, luminescent paint, fire retardant paints, heat resistant paints, varnishes, manufacture of varnishes, enamels, lacquers.

Unit 5 Explosives and Toxic Chemical Weapons

Introduction, Classification. Deflagrating or low explosives. Characteristics of explosives, nitrocellulose, PETN, DNB, TNB, TNT, Picric Acid, Nitroglkycerine, Dynamite, Cirdite, Gun powder, RDX, EDNA, HMX,Tetryl, Pentryl, Hexyl, Dinol. Toxic chemical weapons, screening smokes, Incendiaries, Pyrotechniques, Explosives in India.

TEXTBOOKS:

1. *B.K.Sharma, 'Industrial Chemistry', Goel publishing.*
2. *James A Kent, 'Riegels Hand book of Industrial chemistry', 10th edition, Kluwer Academic/Plenum publishers, 2003.*

REFERENCES

1. *Alan Heaton, 'An Introduction to Industrial chemistry', 3rd edition, Blackie Academic and professional, 1996.*
2. *Chris A Clausen and Guy Mattson, 'Principles of industrial chemistry', 2nd edition Wiley, 1978.*
3. *Jonathan Steed, 'Core Concepts on supramolecular chemistry and nanochemistry', Wiley Eastern Publishers, 2006.*

18CHY637 MEDICINAL CHEMISTRY 3 0 0 3

Course Outcomes

CO1: To understand the physicochemical properties of drug and its metabolic pathways, adverse effect and therapeutic value of drugs.
CO2: To know the role of enzymes and vitamins in biological action.
CO3: To understand the chemistry of various drugs with respect to their pharmacological activity

Skill: After completion of the course the student will attain skill in drug design and medicinal agents.

Unit 1 Medicinal chemistry: Introduction, drugs – classification of drugs – mechanism of drug action. Drug-receptor complex, nomenclature – agonist,

Unit 2 Physicochemical properties of drugs in relation to biological action: solubility**,** Partition coefficient, dissociation constant, hydrogen bonding, ionization, drug shape, surface activity, complexation, protein binding, molar refractivity, bioisosterism – stereo chemical aspects of drug action.
Unit 2: Enzymes, hormones and Vitamins - representative cases, nomenclature, classification and characteristics of enzymes, mechanism of enzyme action, factors affecting enzyme action, co-factors and co-enzymes, enzymes in organic synthesis, mechanism of enzyme catalysis, enzyme inhibition. Hormones and vitamins – representative cases.

Unit 3 Essentials of drug design
Molecular mimetics, drug-lead modification, drug design using QSAR and computer assisted design, assessment of drug activity, receptors and drug action, mechanism of drug action, drug metabolism pathways, Drug potentiation, drug antagonism and drug resistance

Unit 4 Medicinal agents from natural products
History of the use of natural products as therapeutic agents, medicinal plants, active principle, Isolation methods of alkaloids, terpenes, antioxidants, natural oils from plants

Unit 5 Medicinal agents
Medicinal agents belonging to alkaloids, steroids, polypeptides, modified nucleic acid bases, sulphonamide and sulpha drugs, antibacterials - sulpha drugs, substituted sulphonamides, anticonvulsants, anticoagulants, antiamoebic agents, antihelmintic agents, anti-malarial agents, diuretics and cardio vascular agents, , medicinal agents affecting CNS, analgesics, antipyretics, antiseptics and disinfectants, Histamine and anti-histaminic agents. Infectious and non infectious diseases (malaria, AIDS, Cancer) introduction, mechanism of action types of cure,

TEXTBOOKS:

1. *John M beak and John H Block, 'T Wilson, O. Gisvold and R. F. Deorge - Text book of Organic, Medicinal and Pharmaceutical Chemistry', 7th edition, J.B. Lippincott Williams and Wilkons Company, 1977.*
2. *A.Burger, 'Medicinal Chemistry', 3rd edition, Wiley Interscience, 1970.*
3. *V.K.Ahluwalia and Madhu Chopra, 'Medicinal Chemistry', Ane Books pvt Ltd, 2008.*

REFERENCES

1. *V.Kothekar, 'Essentials of Drug Designing', 14th edition, Dhruv publications, 2005.*
2. *V.K.Ahluwalia, Lalita S.Kumar and Sanjiv Kumar, 'Chemistry of Natural Products', Ane Books India.*
3. *L.P.Graham 'An introduction to Medicinal Chemistry', 3rd edition, Oxford University Press, 2005.*

18CHY642 Computational Chemistry 3 0 0 3

Course Outcomes

CO1: Understand the Criteria for modeling the different methods available in computation.
CO2: Understand Quantum mechanical approach and to apply the mathematical skill and knowledge along with quantum mechanical approach to find the characteristics- reactivity, stability, etc., of the molecule and to calculate the energy of a system.
CO3: Ability to get a brief idea about molecular mechanics based calculations.

CO4: Capacity to get an idea about general methodology of molecular modeling.
CO5: Capability to get the basic idea of Density functional theory for the computation.

Skill: Basic knowledge of theoretical calculation involved in computation of Energy for few simple compounds.

Unit 1 - Introduction

Introduction to computational chemistry (molecular modelling), questions commonly investigated computationally, principle and application of methods (tools) of computational chemistry - molecular mechanics, ab initio method, semiempirical methods, density functional theory and molecular dynamics, STOs, GTOs, basis sets, specification of molecular geometry using Cartesian coordinates and internal coordinates, Z-matrix, Z-matrix of simple molecules (water, ethanol), potential energy surface (PES), potential energy surface of diatomic molecules and triatomic molecules (H_2O and HOF) - hypersurface and process of "slicing", stationary points on apotential energy surface - potential energy surface of the isomerization reaction of ozone to isoozone, stationary points (ozone, isoozone and transition state), intrinsic reaction coordinate, minimum, relative minimum, saddle-shaped surface, saddle point, higher-order saddle point and mathematical treatment of stationary points, Born-Oppenheimer approximation and its significance and frozen-nuclei energy.

Unit 2 - Molecular Mechanics

Introduction to molecular mechanics, forcefield, developing a force field - expression for potential energy of a molecule, bond stretching term, angle bending term, torsional term and nonbonded interaction term,parameterizing a forcefield -parameterizingbond stretching term, angle bending term, torsional term and nonbonded interaction term, calculation using forcefield - compare the energies of two 2, 2, 3, 3-tetramethylbutane geometries, illustration of application (use) ofmolecular mechanics - calculation of geometries and energies of small-sized and medium-sized molecules, polymers and transition states (transition state for the Diels-Alder reaction of butadiene with ethene to form cyclohexene), in organic synthesis for predicting the more suitable path for carrying out the synthesis and calculation of normal-mode vibrational frequencies for characterizing a species as a minimum or a transition state or higher-order saddle point, for obtaining zero-point energies to correct frozen-nuclei energies and for interpreting or predicting IR spectra, strength (merit) and weakness (demerit) of molecular mechanics.

Unit 3 - Semiempirical methods - Part 1

Introduction to semiempirical (SE) methods, Simple Huckel Method (SHM) - theory - expression for calculating energy of a molecular species, expression for molecular wave function based on LCAO approximation, secular equations and the single matrix equation, H, C, S and ε matrices and their interpretation, the values of H_{ij} as zero, coulomb integral α and bond integral β and their physical significance, the H matrix in terms of α, β and zero for ethene system(ethene neutral molecule, ethene radical cation and ethene radical anion), propenyl system (propenyl cation, propenyl neutral radical and propenyl anion) and cyclobutadiene system (square cyclobutadiene dication, square cyclobutadiene neutral molecule and square cyclobutadiene dianion), the H matrix in terms of zero, $\alpha = 0$ and $\beta = -1$for ethene systems (ethene neutral molecule, ethene radical cation and ethene radical anion), propenyl system (propenyl cation, propenyl neutral radical and propenyl anion) and cyclobutadiene system (square cyclobutadiene dication, square cyclobutadiene neutral molecule and square cyclobutadiene dianion), result of diagonalization of the H matrices written for ethene system, propenyl system and cyclobutadiene system, molecular orbital energy level diagrams and expressions for energy and molecular wave functionsfor ethene system, propenyl system and cyclobutadiene system based on the result of diagonalization of the H matrices, and molecular orbital energy level diagrams for ethene system,

propenyl system and cyclobutadiene system showing ground state and excited state electronic configurations.

Unit 4 - Semiempirical methods - Part 2

Application of SHM - nodal properties of molecular orbitals and Woodward-Hoffmann orbital symmetry rule, stability towards oxidation and reduction of various species in ethene system, propenyl system and cyclobutadiene system, geometry of cyclobutadiene molecule as predicted by SHM and its Jahn-Teller distortion, aromaticity and Huckel's $(4n + 2)$ π electron rule,and calculation of resonance (stabilizing) energy, bond order and atomic charges of various species in ethene system, propenyl system and cyclobutadiene system, strength of SHM, weakness of SHM (detailed explanation) - basis set is limited to p orbitals (p_z orbitals), it treats only π electrons, and the overlap integrals, Fock matrix elements, electron spin and electron-electron repulsion are not calculated/accounted properly, Extended Huckel Method (EHM) - minimal valence basis set, calculation of Fock matrix elements, and calculation of overlap integrals by Lowdin orthogonalization, EHM procedure, EHM calculation on protonated helium molecule, application of EHM - an overall idea, strength and weakness of EHM, SCF SE methods - Pariser-Parr-Pople (PPP) method and Complete Neglect of Differential Overlap (CNDO) method - basic principle (an exhaustive treatment is **not** expected).

Unit 5 - Density Functional theory and ab initio method

(An exhaustive treatment is **not** expected)

Introduction to Density Functional theory and calculations, Kohn-Sham approach - the first and the second Hohenberg-Kohn theorems, introduction to ab initio method and calculation, basis sets for H, He and first, second and third row elements used in ab initio calculations - STO-3G, 3-21G, 3-21G$^{(*)}$ and 6-31G*****, these basis sets for a few molecular species (water, methane and carbene), basic principles of ab initio method (an idea only).

Text Book

1. Computational Chemistry-Introduction to the Theory and Applications of Molecular and Quantum Mechanics - Errol Lewars

18CHY643 Sustainable Chemical Science 3 0 0 3

Unit 1

Green Chemistry and SustainabilityHistory of green chemistry, Chemical composition of the, environment (Air, water & soil-Role of organic and inorganic molecules in pollution), the twelve principles of green chemistry (detailed description with examples), green chemistry as an expression of envi-ronmental ethics (Thrift Chemistry),the concept of sustainability, from green to sustainable chemistry, sustainable use of chemical feedstock, water and energy, quantifying greenness of a chemical reaction, green chemistry metrics-mass based, energy and environmental metrics,designing greener process, life cycle assessment (introduction and scope),Green toxicology-the need, principles of

toxicology, Disposition of Toxicants in Organisms, Non-Organ Sys-tem Toxicity, Mechanistic Toxicology, Quantitative Structure–Activity Relationships, (Envi-ronmental Toxicology-Persistence and bioaccumulation), Non-Cancer risk assessment, Can-cer risk assessment, stakeholders in sustainable policy implementation.

Unit 2

Chemistry in waterDefinition and attributes of a green solvent, the principle and reasons for use of water in green chemistry-hydrophobicity-cyclodextrin chemistry, Lewis acids in aqueous media, Michael addition in water using triflates, green processes with base in water, green oxida-tions and reduction in water, on water conditions, use of water in microwave and ultrasonic technology.

Unit 3

Green solventsIonic liquids as green solvents-definitionand notation-properties, synthesis and use in organic reactions, oxidation, oxidative carbonylation of aniline,Friedel–crafts reaction, Michael addition, Fischer Indole synthesis, Benzoin condensation, dimethyl carbonates syn-thesis in ionic liquids.Super critical fluids-super critical water and carbondioxide-properties and organic transformations.(Diels Alder, Clasen rearrangement, Fisher Indole, Friedel–crafts reaction, oxidation and hydrogenation.Properties and application in organic transformation of green solvents like polyeth-ylene glycol, glycerol, cyclopentyl methyl ether, 2-methyltetrahydro furan, Perfluorinated (Fluorous) Solvents-FluorousBiphase Concept and dimethyl carbonate.

Unit 4

Green Chemistry and CatalysisImportance of catalysis, turn over number and frequency, the basis of catalysis-kinetic phenomenon, basics of homogeneous, heterogeneous and biocatalysis, sabatier's principle, catalyst -deactivation, sintering, thermal degradation, inhibition and poisoning, cat- alyst promoters, modifiers, supported catalysts and reagents for green chemistry-heterogen-ized reactions for green chemistry, preparation of solid catalyst-slurry and co-precipitation, impregnation, hydrothermal synthesis-drying, calcination, activation and forming, selecting the right support, catalyst characterization-surface characterization methods, temperature programmed techniques, spectroscopyand microscopy.Common mechanism in enzyme ca-talysis immobilized enzymes, developing biocatalyst-rational design and directed evolution, non-enzymatic biocatalysts.

Unit 5 Green Chemistry Technologies and Alternate Energy SourcesDesign for Energy Efficiency, Photochemical Reactions Advantages of and Challenges Faced by Photochemical Processes

(Examples)Microwaves as energy source in chemistry-properties of microwaves, microwave heating (Effects), Approaches to Microwave-assisted Organic Chemistry-solvent free meth-ods, MORE chemistry, continuous microwave reactor (CMR)-microwave batch reactor (MBR), examples of organic transformations.Sonochemistry and Green Chemistry-Theoretical Basis-Cavitation Inception, Nu-cleation-Bubble Dynamics-examples of organic transformations, Sono-chemical synthesis of nano-structured materials, Electrochemical Synthesis-materials manufactured using the process, organic elec-trosynthesis-3-bromothiophen from thiopheneRenewable Sources of Energy, Solar Energy, Wind Power, Geothermal Solution, Hy-dropower (Sources, Merits and Difficulties in widespread applications), Indian Energy sce-nario-Energy Conservation act (2001)-features.

Reference

1.Green chemistry and engineering A Pathway to Sustainability, Anne E. Marteel-Parrish, Martin A. Abraham, American Institute of Chemical Engineers, Inc, John Wiley & Sons, Inc 2014.

2.Synthetic organic Sonochemistry, Jean-Louis luche, Springer Science+Business Me-dia New York, 1998

3.New Methodologies and Techniques for a Sustainable Organic Chemistry, Ales-sandro Mordini and FerencFaigl, Springer, 2008.

4.Green chemistry, Fundamentals and Applications, Suresh C. Ameta and RakshitAme-ta, CRC press, Taylor & Francis Group, 2013

5.Handbook of Green Chemistry, Vol5 Green Solvents-Reactions in Water, PualT An-astas, Chao Jun Li

6.Sonochemistry: theory, reactions, syntheses, and applications, Filip M. Nowak, Nova Science Publishers, Inc, 2010.

7.Green Chemistry Metrics, A Guide to Determining and Evaluating Process Green-ness, Dicks, Andrew, Hent,Andrei, SpringerBriefs in Green Chemistry for Sustaina-bility, 2015

8.Catalysis: concepts and applications, Gadi Rothenberg,Wiley-VCH Verlag& Co. KGaA, Weinheim, Germany, 2008

18CHY633 CHEMISTRY OF BIOMOLECULES 3 0 0 3

Course Outcomes

CO1: Understand the role of aminoacids, proteins and peptides in biology along with their application.

CO2: Able to describe the basic properties, mechanisms of action and applications of enzymes
CO3: Gain knowledge in nucleic acids, antibodies, recombtinant DNAand gene analyses.

Unit 1 Amino acids, Proteins and Peptides
Classification, Stereochemical aspects, physical properties, Ionic properties, spectral properties, essential and non essential amino acids, chemical reactions of amino acids, Industrial preparation and chemical synthesis of amino acids. Ionic properties of proteins, protein structure, protein purification, protein structure determination, proteomics and protein function, solid phase peptide synthesis, biologically important peptides.

Unit 2 Enzymes Introduction to Enzymes, Classification of enzymes, mechanism of enzyme action, immobilized enzymes and enzyme technology, enzyme analog built polymers, design of molecular clefts, enzymes in synthetic organic chemistry. Enzymes in biological systems

Unit 3 Molecular biology and bioinformatics
Structure of nucleic acids, genes and genome complexity, functions of nucleic acids, isolation and separation of nucleic acids, molecular analysis of nucleic acid sequences, nucleotide sequencing of DNA.

Unit 4 Immunochemical techniques
Production of antibpodies, purification and fragmentation of immunoglobulins, immunoprecipitatipon, labeling antibodies, immunoblotting, immunoassays, immunohisto/cytochemistry.

Unit 5 Recombinant DNA and genetic analysis
Constructing gene libraries, cloning vectors, hybridization and gene probes, application of gene cloning, expression of foreign genes, pharmacogenomics.

REFERENCES:

3. *Hermann Dugas, 'Bioorganic Chemistry - A Chemical Approach to Enzyme Action', 3rd edition, Springer.*
4. *Keith Wilson and John Walker, 'Principles and Techniques of Biochemistry and Molecular Biology', 6th edition, Cambridge University Press.*

18CHY634 INDUSTRIAL CHEMISTRY 3 0 0 3

Course Outcomes

CO1: To gain knowledge about various water treatment processes adopted in industries

CO2: To provide in-depth overview on production, refining and processing of various types of fuels

CO3: To understand the importance and preparative methods of explosives and chemical weapons
CO4: To learn the manufacturing process of paints and pigments and to develop ability to scale up the products prepared in the laboratory to the industrial level
CO5: To obtain a comprehensive knowledge of various energy resources used commercially
CO6: To calculate, analyse and execute different types of industrial processes

Unit 1 Water treatment
Softening of water, Ion exchange process, Lime soda process, Modified Lime soda process, Zeolite process, Chemical and physical method of sterilization, Desalination, Boiler problems. Corrosion of boiler units, industrial water treatment, water analysis.

Unit 2 Fuels
Calorific value, determination of Calorific value, classification of fuels, Solid fuels, Properties of fuels, classification of coal, coking and non-coking coals, advantages and disadvantages of solid fuels. Liquid fuels, gaseous fuels, analysis of fuel gases, Distillation of petroleum. Processing & purification of petroleum and petroleum products, Flash point, Fire point, Knocking, antiknocking, Cetane number, octane number, natural gasoline, cracking, polymerization, alkylation, isomerisation, rocket fuels, fossil fuel, nuclear fuels.

Unit 3 Energy resources
Renewable and non renewable sources of energy, conventional and non conventional sources of energy, solar energy, solar technology, solar photovoltaic cell - application, PV lantern system, Radiotelephone system, Application of solar energy, Environmental implication, Nuclear energy, nuclear fuel cycle in India, Energy conservation and waste heat boilers, Fuel cells, hydrogen cells.

Unit 4 Paints and Pigments
White pigment, blue, green, yellow, black and red pigments - manufacture, physical properties, characteristics, Manufacture of paints, setting of paints, requirement for good paints, emulsion paint, latex paint, luminescent paint, fire retardant paints, heat resistant paints, varnishes, manufacture of varnishes, enamels, lacquers.

Unit 5 Explosives and Toxic Chemical Weapons
Introduction, Classification. Deflagrating or low explosives. Characteristics of explosives, nitrocellulose, PETN, DNB, TNB, TNT, Picric Acid, Nitroglkycerine, Dynamite, Cirdite, Gun powder, RDX, EDNA, HMX,Tetryl, Pentryl, Hexyl, Dinol. Toxic chemical weapons, screening smokes, Incendiaries, Pyrotechniques, Explosives in India.

TEXTBOOKS:

3. *B.K.Sharma, 'Industrial Chemistry', Goel publishing.*
4. *James A Kent, 'Riegels Hand book of Industrial chemistry', 10th edition, Kluwer Academic/Plenum publishers, 2003.*

REFERENCES

4. *Alan Heaton, 'An Introduction to Industrial chemistry', 3rd edition, Blackie Academic and professional, 1996.*
5. *Chris A Clausen and Guy Mattson, 'Principles of industrial chemistry', 2nd edition Wiley, 1978.*
6. *Jonathan Steed, 'Core Concepts on supramolecular chemistry and nanochemistry', Wiley Eastern Publishers, 2006.*

18CHY637 MEDICINAL CHEMISTRY 3 0 0 3

Course Outcomes

CO1: To understand the physicochemical properties of drug and its metabolic pathways, adverse effect and therapeutic value of drugs.

CO2: To know the role of enzymes and vitamins in biological action.

CO3: To understand the chemistry of various drugs with respect to their pharmacological activity

Unit 1 Medicinal chemistry: Introduction, drugs – classification of drugs – mechanism of drug action. Drug-receptor complex, nomenclature – agonist,

Unit 2 Physicochemical properties of drugs in relation to biological action: solubility**,** Partition coefficient, dissociation constant, hydrogen bonding, ionization, drug shape, surface activity, complexation, protein binding, molar refractivity, bioisosterism – stereo chemical aspects of drug action.

Unit 2: Enzymes, hormones and Vitamins - representative cases, nomenclature, classification and characteristics of enzymes, mechanism of enzyme action, factors affecting enzyme action, co-factors and co-enzymes, enzymes in organic synthesis, mechanism of enzyme catalysis, enzyme inhibition. Hormones and vitamins – representative cases.

Unit 3 Essentials of drug design

Molecular mimetics, drug-lead modification, drug design using QSAR and computer assisted design, assessment of drug activity, receptors and drug action, mechanism of drug action, drug metabolism pathways, Drug potentiation, drug antagonism and drug resistance

Unit 4 Medicinal agents from natural products

History of the use of natural products as therapeutic agents, medicinal plants, active principle, Isolation methods of alkaloids, terpenes, antioxidants, natural oils from plants

Unit 5 Medicinal agents

Medicinal agents belonging to alkaloids, steroids, polypeptides, modified nucleic acid bases, sulphonamide and sulpha drugs, antibacterials - sulpha drugs, substituted sulphonamides,

anticonvulsants, anticoagulants, antiamoebic agents, antihelmintic agents, anti-malarial agents, diuretics and cardio vascular agents, , medicinal agents affecting CNS, analgesics, antipyretics, antiseptics and disinfectants, Histamine and anti-histaminic agents. Infectious and non infectious diseases (malaria, AIDS, Cancer) introduction, mechanism of action types of cure,

TEXTBOOKS:

4. *John M beak and John H Block, 'T Wilson, O. Gisvold and R. F. Deorge - Text book of Organic, Medicinal and Pharmaceutical Chemistry', 7th edition, J.B. Lippincott Williams and Wilkons Company, 1977.*
5. *A.Burger, 'Medicinal Chemistry', 3rd edition, Wiley Interscience, 1970.*
6. *V.K.Ahluwalia and Madhu Chopra, 'Medicinal Chemistry', Ane Books pvt Ltd, 2008.*

REFERENCES

4. *V.Kothekar, 'Essentials of Drug Designing', 14th edition, Dhruv publications, 2005.*
5. *V.K.Ahluwalia, Lalita S.Kumar and Sanjiv Kumar, 'Chemistry of Natural Products', Ane Books India.*
6. *L.P.Graham 'An introduction to Medicinal Chemistry', 3rd edition, Oxford University Press, 2005.*

18CHY642 Computational Chemistry 3 0 0 3

Course Outcomes

CO1: Understand the Criteria for modeling the different methods available in computation.
CO2: Understand Quantum mechanical approach and to apply the mathematical skill and knowledge along with quantum mechanical approach to find the characteristics- reactivity, stability, etc., of the molecule and to calculate the energy of a system.
CO3: Ability to get a brief idea about molecular mechanics based calculations.
CO4: Capacity to get an idea about general methodology of molecular modeling.
CO5: Capability to get the basic idea of Density functional theory for the computation.

Unit 1 - Introduction

Introduction to computational chemistry (molecular modelling), questions commonly investigated computationally, principle and application of methods (tools) of computational chemistry - molecular mechanics, ab initio method, semiempirical methods, density functional

theory and molecular dynamics, STOs, GTOs, basis sets, specification of molecular geometry using Cartesian coordinates and internal coordinates, Z-matrix, Z-matrix of simple molecules (water, ethanol), potential energy surface (PES), potential energy surface of diatomic molecules and triatomic molecules (H_2O and HOF) - hypersurface and process of "slicing", stationary points on apotential energy surface - potential energy surface of the isomerization reaction of ozone to isoozone, stationary points (ozone, isoozone and transition state), intrinsic reaction coordinate, minimum, relative minimum, saddle-shaped surface, saddle point, higher-order saddle point and mathematical treatment of stationary points, Born-Oppenheimer approximation and its significance and frozen-nuclei energy.

Unit 2 - Molecular Mechanics

Introduction to molecular mechanics, forcefield, developing a force field - expression for potential energy of a molecule, bond stretching term, angle bending term, torsional term and nonbonded interaction term,parameterizing a forcefield -parameterizingbond stretching term, angle bending term, torsional term and nonbonded interaction term, calculation using forcefield - compare the energies of two 2, 2, 3, 3-tetramethylbutane geometries, illustration of application (use) ofmolecular mechanics - calculation of geometries and energies of small-sized and medium-sized molecules, polymers and transition states (transition state for the Diels-Alder reaction of butadiene with ethene to form cyclohexene), in organic synthesis for predicting the more suitable path for carrying out the synthesis and calculation of normal-mode vibrational frequencies for characterizing a species as a minimum or a transition state or higher-order saddle point, for obtaining zero-point energies to correct frozen-nuclei energies and for interpreting or predicting IR spectra, strength (merit) and weakness (demerit) of molecular mechanics.

Unit 3 - Semiempirical methods - Part 1

Introduction to semiempirical (SE) methods, Simple Huckel Method (SHM) - theory - expression for calculating energy of a molecular species, expression for molecular wave function based on LCAO approximation, secular equations and the single matrix equation, H, C, S and ε matrices and their interpretation, the values of H_{ij} as zero, coulomb integral α and bond integral β and their physical significance, the H matrix in terms of α, β and zero for ethene system(ethene neutral molecule, ethene radical cation and ethene radical anion), propenyl system (propenyl cation, propenyl neutral radical and propenyl anion) and cyclobutadiene system (square cyclobutadiene dication, square cyclobutadiene neutral molecule and square cyclobutadiene dianion), the H matrix in terms of zero, $\alpha = 0$ and $\beta = -1$for ethene systems (ethene neutral molecule, ethene radical cation and ethene radical anion), propenyl system (propenyl cation, propenyl neutral radical and propenyl anion) and cyclobutadiene system (square cyclobutadiene dication, square cyclobutadiene neutral molecule and square cyclobutadiene dianion), result of diagonalization of the H matrices written for ethene system, propenyl system and cyclobutadiene system, molecular orbital energy level diagrams and expressions for energy and molecular wave functionsfor ethene system, propenyl system and cyclobutadiene system based on the result of diagonalization of the H matrices, and molecular orbital energy level diagrams for ethene system, propenyl system and cyclobutadiene system showing ground state and excited state electronic configurations.

Unit 4 - Semiempirical methods - Part 2

Application of SHM - nodal properties of molecular orbitals and Woodward-Hoffmann orbital symmetry rule, stability towards oxidation and reduction of various species in ethene system, propenyl system and cyclobutadiene system, geometry of cyclobutadiene molecule as predicted by SHM and its Jahn-Teller distortion, aromaticity and Huckel's (4n + 2) π electron rule,and calculation of resonance (stabilizing) energy, bond order and atomic charges of various species in ethene system, propenyl system and cyclobutadiene system, strength of SHM, weakness of SHM (detailed explanation) - basis set is limited to p orbitals (p_z orbitals), it treats only π electrons, and the overlap integrals, Fock matrix elements, electron spin and electron-electron repulsion are not calculated/accounted properly, Extended Huckel Method (EHM) - minimal valence basis set, calculation of Fock matrix elements, and calculation of overlap integrals by Lowdin orthogonalization, EHM procedure, EHM calculation on protonated helium molecule, application of EHM - an overall idea, strength and weakness of EHM, SCF SE methods - Pariser-Parr-Pople (PPP) method and Complete Neglect of Differential Overlap (CNDO) method - basic principle (an exhaustive treatment is **not** expected).

Unit 5 - Density Functional theory and ab initio method

(An exhaustive treatment is **not** expected)

Introduction to Density Functional theory and calculations, Kohn-Sham approach - the first and the second Hohenberg-Kohn theorems, introduction to ab initio method and calculation, basis sets for H, He and first, second and third row elements used in ab initio calculations - STO-3G, 3-21G, 3-21G$^{(*)}$ and 6-31G**, these basis sets for a few molecular species (water, methane and carbene), basic principles of ab initio method (an idea only).

Text Book

1. Computational Chemistry-Introduction to the Theory and Applications of Molecular and Quantum Mechanics - Errol Lewars