SYLLABUS

For

M. Sc. Course in

Chemistry

To be effective from the session 2016-17

KAZI NAZRUL UNIVERSITY

ASANSOL 713 340

WEST BENGAL, INDIA

Duration of PG Course of Studies in Chemistry will be of two years with four Semesters, viz., Semester I, Semester II, Semester III and Semester IV - each of six months' duration coupled with four examinations *viz.* Semester I, Semester II, Semester III and Semester IV in chemistry at the end of each Semester. Syllabus is hereby framed according to certain schemes and structures highlighted below.

Schemes:

(i) 300 marks in Semester I & III, 350 marks for Semester II and 250 marks for Semester IV with a grand total of 1200 marks and 98 credits.

(ii) 24 credits in Semester I & III, 28 credits in Semester II and 22 credits in Semester IV with a total of 98 credits; each theoretical/practical paper of 4 credits; term paper/project of 6 credits;

(iii) 20% marks allotted for internal assessment in each paper

(iv) Four theoretical general papers (common to all students) in each of Semester I and Semester II

(v) Two practical general papers (common to all students) in each of Semester I and Semester II

(vi) Three major electives *viz.* Inorganic, Organic and Physical in Semester III and Semester IV; number of students in each Major paper to be decided by the department; the particular major paper once chosen by any student in Semester III, the corresponding major paper to be continued in Semester IV

(vii) For theoretical papers in Semester III, three advanced general papers (common to all students) and one major paper

(viii) For practical papers in Semester III, one advanced general paper strictly on instrumental methods in chemical analysis with computer simulation (common to all students) and one Major paper (applicable to students as selected by department)

(ix) For theoretical papers in Semester IV, one advanced general paper (common to all students) and two major papers (applicable to students as per provision made in Semester III by the department)

(x) For practical paper in Semester IV, one major practical paper (applicable to students as selected by department)

(xi) In Semester II, one Extra Departmental elective paper to be learnt by the students of the other sister departments and the students of this department be learnt from other sister departments.

(xii) In Semester IV, one paper on term paper/project work (subject matter of each major paper of Semester IV)

(xii) In all semesters each theoretical paper consisting of two units, viz., Unit I and Unit II

(xiii) Total eight questions each with 8 marks to be set in each theoretical paper with each unit containing four questions; examinees to be answered a total of five questions taking at least two from each Unit

(xiv) Duration of examination: each theoretical paper of 50 marks, each practical paper, 6 hours

(xv) For each practical paper: internal assessment, 10; experiments, 30; viva-voce (by external examiner), 10

(xvi) For term paper/project work: internal assessment, 10; presentation of seminar in presence of external expert; 30, and thereafter interaction, 10

Course Structure

SEMESTER I	Paper Code	Core Subject	Marks*	Credit**
	Theoretical Papers			
	MSCCHEMC101	Inorganic Chemistry General - I	50	4
	MSCCHEMC102	Organic Chemistry General I	50	4
	MSCCHEMC103	Physical Chemistry General I	50	4
	MSCCHEMC104	Analytical Chemistry General I	50	4
	Practical Papers			
	MSCCHEMC105	Inorganic Chemistry General: Practical	50	4
	MSCCHEMC106	Organic Chemistry General: Practical	50	4
		Total	**300**	**24**

SEMESTER II	Paper Code	Core Subject	Marks*	Credit**
	Theoretical Papers			
	MSCCHEMC201	Inorganic Chemistry General II	50	4
	MSCCHEMC202	Organic Chemistry General II	50	4
	MSCCHEMC203	Physical Chemistry General II	50	4
	MSCCHEMC204	Analytical Chemistry General II	50	4
	Practical Papers			
	MSCCHEMC205	Physical Chemistry General: Practical	50	4
	MSCCHEMC206	Analytical Chemistry General: Practical	50	4
	Extra Departmental Elective#			
	MSCCHEMMIE201	Supramolecular and Medicinal Chemistry	50	4
		Total	**350**	**28**

SEMESTER III	Paper Code	Core Subject	Marks*	Credit**
	Theoretical Papers			
	MSCCHEMC301	Advanced Inorganic Chemistry General	50	4
	MSCCHEMC302	Advanced Organic Chemistry General	50	4
	MSCCHEMC303	Advanced Physical Chemistry General	50	4
	Major Electives (any one)			
	MSCCHEMMJE301	Inorganic Chemistry Major I	50	4
	MSCCHEMMJE302	Organic Chemistry Major I	50	4
	MSCCHEMMJE303	Physical Chemistry Major I	50	4
	Practical Papers (MSCCHEMC304 compulsory, and any one from MSCCHEMMJE304-306)			
	MSCCHEMC304	Advanced Chemistry General	50	4
	MSCCHEMMJE304	Inorganic Chemistry Major: Practical I	50	4
	MSCCHEMMJE305	Organic Chemistry Major: Practical I	50	4
	MSCCHEMMJE306	Physical Chemistry Major: Practical I	50	4
		Total	**300**	**24**

	Paper	Core Subject	Marks*	Credit**
S E M E S T E R IV	**Theoretical Papers**			
	MSCCHEMC401	Advanced Analytical Chemistry General	50	4
	Major Electives (any one from MSCCHEMMJE401-403 and any one from MSCCHEMMJE404-406)			
	MSCCHEMMJE401	Inorganic Chemistry Major II	50	4
	MSCCHEMMJE402	Organic Chemistry Major II	50	4
	MSCCHEMMJE403	Physical Chemistry Major II	50	4
	MSCCHEMMJE404	Inorganic Chemistry Major III	50	4
	MSCCHEMMJE405	Organic Chemistry Major III	50	4
	MSCCHEMMJE406	Physical Chemistry Major III	50	4
	Major Elective Practical (any one)			
	MSCCHEMMJE407	Inorganic Chemistry Major: Practical II	50	4
	MSCCHEMMJE408	Organic Chemistry Major: Practical II	50	4
	MSCCHEMMJE409	Physical Chemistry Major: Practical II	50	4
	Term Paper/Project[##] (*any one from MSCCHEMC402-404*)			
	MSCCHEMC402	Inorganic Chemistry Term Paper/Project	50	6
	MSCCHEMC403	Organic Chemistry Term Paper/Project	50	6
	MSCCHEMC404	Physical Chemistry Term Paper/Project	50	6
		Total	**250**	**22**
		Grand Total	**1200**	**98**

* Marks: Sem I + Sem II + Sem III + Sem IV = 300 + 350 + 300 + 250 = 1200;

**Credit: Sem I + Sem II + Sem III + Sem IV = 24 + 28 + 24 + 22 = 98;

[#] Number of students-intake for minor electives may depend on the availability of seats;

[##] For term paper/project: preparation + presentation + viva-voce = 25 + 15 + 10 = 50.

Programme Overview

Duration: 2 Years | Programme Code: MSCCHEM

Master of Science (M.Sc.) in Chemistry offers a wide range of courses including Inorganic Chemistry, Organic Chemistry, Medicinal Chemistry, Supramolecular Chemistry, etc. Experts from Pure and Applied Chemistry domain will teach the courses, and students will develop a thorough understanding of fundamentals and experimental concepts of Chemistry. There will be opportunity for the students to participate in an extensive and varied seminar programme and gain experience in a large variety of projects.

Programme Educational Objectives

- The graduates will become successful professional by demonstrating logical and analytical thinking abilities.
- The graduates will work and communicate effectively in interdisciplinary environment, either independently or in team, and demonstrate scientific leadership in academia and industry.
- The graduates will engage in lifelong learning and professional development through discussion, professional and doctoral level studies.

Programme Outcomes

At the end of the programme the students will be able to:

- Acquire knowledge, abilities and insight in well-defined area of research within Chemistry.
- Work as a Chemistry professional, and qualify for training as scientific researcher.
- Develop knowledge of scientific theories and methods, gain experience in working independently with scientific questions and clearly express their opinion on academic issues.
- Develop communication skills, both written and oral, for specialized and non-specialized audiences.
- Acquire the skills of planning and conducting advanced chemical experiments and applying structural-chemical characterization techniques.
- Examine specific phenomena theoretically and/or experimentally, contribute to the generation of new scientific insights or to the innovation of new applications of research in Chemistry.

Programme Highlights

- Distinctive academic curriculum, qualified and competent faculty members, transfer of knowledge through scholarly activities, Interdisciplinary project based learning, state-of-the-art laboratories, exceptional computational facilities, industry interaction, and semester abroad opportunities.

Some of the major areas that will be covered

- Inorganic Chemistry, Physical Chemistry, Organic Chemistry, Medicinal Chemistry, Supramolecular Chemistry, Instrumental Methods of Analysis, Co-ordination and Organometallic Chemistry, Organic Synthesis and Reagents, Quantum Chemistry and Group Theory, Natural Product Chemistry, Numerical Methods and Computer Programming, and project based learning.

Career Avenues

- Chemistry is used in medicine, natural sciences, technology, environment, and much more. Graduates with Master's degrees in Chemistry are in demand on the job market in sectors ranging from energy to environment, teaching to research, pharmaceutical to medical sciences.

Entry Requirements

- An undergraduate degree in a related discipline from UGC approved University. B.Sc. with honours in chemistry degree will be preferred.

Semester I

Theoretical Papers (For Each, Full Marks: 50; Credit: 4)

MSCCHEMC101: Inorganic Chemistry General I

Course Objective:

Today nuclear chemistry is a part of our course curriculum and has been introduced with an objective to present a vignette of the composition of the nuclear structure, its stability and induce the students to take up nuclear research in their higher studies. Students should have basic ideas of coordination chemistry, organometallic chemistry, bioinorganic and inorganic medicinal chemistry etc. There are lots of scope and opportunities, research and development in this subject, since a lot still remains unexplored in this arena.

Learning Outcomes:

Explain the macroscopic observables associated with nuclear change and the microscopic or chemists view of nuclear change. Identify and define various types of nuclear changes or processes including fission, fusion and decay reactions. Use proper isotopic notation to write down and balance a nuclear reaction. State and compare the differences and similarities between a nuclear change and a chemical change.

Unit I

1. Bonding, reactivity and molecular properties – a quantum chemical approach (12 lectures)

Fundamentals, LCAO and/or Huckel treatments of σ-and π-MOs (inorganic di-/polyatomic species, organic open-chain/cyclic units such as alkanes, alkenes, vinylic/allylic system, dienes, polyenes, sandwich molecules, boron/carborane compounds, etc) with an inner look into orbital symmetry, molecular term symbols, relative energy, transition probability, selection rules, nature and intensity of transitions (allowed/forbidden), probing reaction center, and aromaticity of inorganic, organic, coordination and organometallic species; Koopmans' theorem, Walsh diagram, isolobal analogy

2. Coordination chemistry – stereochemistry, bonding and structure (13 lectures)

Preamble, Orgel/Tanabe-Sugano diagram, ligand symmetry orbital, molecular orbital, Angular overlap model, spectral features, Nephelauxetic effect, Racah parameter, Franck Condon principle, vibronic coupling, band broadening, spin-orbit coupling, spin-forbidden transition, intensity stealing, magnetic properties, cooperative, anomalous and subnormal magnetic moments, lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, conformation of chelator/congregator/macrocycle, structural equilibrium and implication

Unit II

3. Organometallic chemistry I (10 lectures)

Overview, valence electron count, oxidation number and formal ligand charge; carbonyl ligand, linear/cyclic π- ligand system, compounds with M-C, M=C and M≡C bonds, hydride and dihydrogen complexes; phosphine, Jesiphos and related ligands; spectral analysis and structural characterization, Dewar-Chatt-Duncanson bonding model, isolobal analogy, Agostic interaction

4. Bioinorganic and inorganic medicinal chemistry (15 lectures)

Background, myoglobin, heamoglobin, heamocyanin, hemerythrin, cytochromes, rubredoxin, feredoxins; biological nitrogen fixation, chlorophyll and photosynthesis; PS-I, PS-II, bioenergetics and ATP cycle, glucose storage, Na^+/K^+ ion pump, ionophores, metalloenzyme – catalase, peroxidase, ceruloplasmin, cytochrome oxidase, carbonic anhydrase, carboxy peptidase, metallothionine, xanthine oxidase, sulphite oxidase, nitrate reductase, superoxide dismutase, chemistry of respiration; vitamin B_{12} and B_{12}-enzyme

Metals in medicines: diseases due to deficiencies, carcinogenesis, applications of chelators and metal chelates of different generations; antitumour, anticancer and anti-AIDS drugs, mechanistic pathway, limitation, future dimension

Suggested books

C. J. Ballhausen, *Molecular Electronic Structure of Transition Metal Complexes*, McGraw-Hill, London, 1979.

A. B. P Lever, *Inorganic Electronic Spectroscopy*, Elsevier, New York, 1984.

B. E. Douglas and C. A. Hollingsworth, *Symmetry in Bonding and Spectra*, *An Introduction*, Academic Press, New York, 1985.

T. A. Albright, J. K. Burdett and M. H. Whangbo, *Orbital Interactions in Chemistry*, Wiley, New York, 1985.

K. Fukui and H. Fujimoto, *Frontier Orbital and Reaction Paths*, World Scientific, Singapore, 1995.

J. G. Verkade, *A Pictorial Approach to Molecular Bonding*, 2^{nd} Edn, Springer-Verlag, New York, 1997.

A. Vincent, *Molecular Symmetry and Group Theory*, John Wiley & Sons, New York, 1998.

F. A. Cotton, *Chemical Applications of Group Theory*, 3^{rd} Edn, John Wiley & Sons, New York, 1999.

F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6^{th} Edn, John Wiley & Sons, Inc, New York, 1999.

B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3^{rd} Edn, John Wiley & Sons, Inc., New York, 2001.

G. Wulfsberg, *Inorganic Chemistry*, Viva Books Pvt Ltd, New Delhi, 2001.

J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorgnic Chemistry: Principles of Structures and Reactivity*,

4^{th} Edn, Pearson, New Delhi, 2006.

D. A. McQuarrie, P. A. Rock and E. B. Gallogly, *General Chemistry*, 4^{th} Edn, University Science Books, Mill Valley, Canada, 2011.

C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1994.

D. N. Sathyanarayana, *Electronic Absorption Spectroscopy and Related Techniques*, University Press,2001.
M. Cox, *Optical Properties of Solids*, Oxford University Press, Oxford, 2001.
G. Aruldhas, *Molecular Structure and Spectroscopy*, 2nd Edn, Prentice-Hall of India, New Delhi, 2007.
P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Shriver & Atkins Inorganic Chemistry*, 4th Edn, Oxford, 2006.
I. Pelant and J. Valenta, *Luminescence Spectroscopy of Semiconductors*, Oxford, New York, 2012.
O. Kahn, *Molecular Magnetism*, VCH, New York, 1993.
P. Powell, *Principles of Organometallic Chemistry*, 2nd Edn, Chapman and Hall, London, 1988.
J. D. Atwood, *Inorganic and Organometallic Reaction Mechanisms*, 2nd Edn, VCH, New York, 1997.
A. F. Hill, *Organotransition Metal Chemistry*, Royal Society of Chemistry, London, 2002.
R. H. Crabtree, *The Organomettalic Chemistry of the Transition Metals*, 4th Edn, Wiley, New York , 2005.
C. Elschenbroich, *Organometallics*, 3rd Edn, Wiley-VCH, Weinheim, 2006.
R. A. van Santen and M. Neurock *Molecular Heterogenous Catalysis*, Wiley-VCH, Weinheim, 2006.
G. O. Spessard and G. L. Miessler, *Organometallic Chemistry*, International 2nd Edn, Oxford University Press, Oxford, 2010.
J. F. Hartwig, *Organotransition Metal Chemistry. From Bonding to Catalysis*, University Science Books, Sausalito, CA, 2010.
S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, Mill Valley, CA, 1993.
W. Kaim and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life,* Wiley, New York, 1994.
I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, *Bioinorganic Chemistry*, Viva Books Pvt. Ltd., New Delhi, 1998.
E. Ochiai, *Bioinorganic Chemistry: A Survey*, Academic Press, Elsevier, 2009.
R. R. Crichten, *Biological Inorganic Chemistry:A New Introduction to Molecular Structure*, 2nd Edn, Elsevier, New York, 2012.
R. M. Roat-Malone, *Bioinorganic Chemistry: A short Course*, 2nd Edn, Wiley, New York, 2013.
G. L. Patrik, *An Introduction to Medicinal Chemistry,* 3rd Edn, Oxford University Press, 2006.
C. G. Wermuth (Ed), *The Practice of Medicinal Chemistry*, Academic Press, Noida, India, 2008.

MSCCHEMC102: Organic Chemistry General I

Course Objectives: To learn and apply various concepts such as stereochemistry and fundamental principles of stereoselectivity in organic chemistry. Students should learn also basic organic reaction mechanism and basic organic spectroscopy.

Learning Outcomes: At the end of the course, the learners should be able to: Identify and differentiate prochirality and chirality at centers, axis, planes and helices and determine the absolute configuration. Evaluate the stability of various conformers of acyclic and cyclic systems using steric, electronic and stereoelectronic effects and correlate them to reactivity. Use various models for determining stereoselectivity of various organic transformations. Determine the symmetry operations of any small and medium-sized molecule and apply point group theory to the study of electrical, optical and magnetic properties and selection rules for absorption.

Unit I

1. Stereochemistry (Static and Dynamic) of organic compounds: concept and application (10 lectures)

Static stereochemistry: Molecular symmetry and chirality; axial chirality, planar chirality and helicity; topicity and prostereoisomerism; conformation of acyclic and cyclic systems (3 to 5 and 7 to 8 members ring) along with fused and bridged ring compounds; conformations of rings with multiple double bonds; stereoelectronic effects; Baldwin's rule, stereochemistry of fused ring and bridged ring compounds (with special reference to decalin and phenanthrene systems)

Dynamic stereochemistry: Curtin-Hammett principle and Wenstein-Eliel equations;conformation, reactivity & mechanism (*viz*.acyclic and cyclic system focusing on nucleophilic substitution reaction, formation and cleavage of epoxide ring, addition reactions to double bonds, elimination reactions, pyrolytic *syn*-elimination, oxidation of cyclohexanols,*etc*.);elementary idea about asymmetric synthesis

2. Organic reaction mechanism (15 lectures)

Substitution reactions: Aliphatic nucleophilic substitution — S_N1, S_N2, mixed S_N1 and S_N2, SET mechanisms; neighbouring group participation by *pi*- and *sigma*-bonds, anchimeric assistance; S_Ni mechanism; nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon; effect of substrate structures on reactivity, nucleophiles, leaving group and reaction medium; phase transfer catalysis, regioselectivity; Aromatic nucleophilic substitution — S_NAr, benzyne and $S_{RN}1$ mechanisms; effect of substrate structures on reactivity, leaving group and attacking nucleophile; Aliphatic electrophilic substitution — S_E1, S_E2, and S_E^i mechanisms; electrophilic substitution accompanied by double bond shifts; effects of substrates, leaving group and solvent polarity on the reactivity, Aromatic electrophilic substitution — the arenium ion mechanism; orientation and reactivity; energy profile diagrams; the *ortho*/*para*ratio; orientation in other ring systems; *ipso* attack; *Free radical reactions*: Types of free radical reactions; free radical substitution mechanism; mechanism at an aromatic substrate; neighbouring group assistance; reactivity for aliphatic and aromatic substrates at a bridgehead; reactivity in the attacking radicals; effects of solvents on reactivity; allyllic halogenation (NBS), oxidation of aldehydes to carboxylic acids; auto-oxidation; free radical rearrangements

Elimination reactions: E1, E2 and E1cB mechanisms; product stereochemistry; effects of substrate structures, attacking base, leaving group and the medium on reactivity; mechanism and orientation in pyrolytic elimination

Addition reactions: Addition to carbon–carbon multiple bonds — mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals; region- and chemoselectivity; orientation and reactivity; Addition to carbon–hetero multiple bonds — mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles; addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds; Mechanism of condensation reactions involving enolates — Aldol, Knoevenagel, Claisen, Perkin and Stobbe reactions

Rearrangement reactions: Formation and stability of carbonium ions, carbanion, carbenes, nitrenes, radicals and arynes. Rearrangement involving carbocation (Wagner-Meerwein, Pinacol-Pinacolone rearrangement), reaction involving acyl cation, PPA cyclization and Fries rearrangement, rearrangement of carbenes (Wolff & Arndst-Eistert synthesis), rearrangement of nitrenes (Hoffmann, Curtius, Schmidt, Lossen, Beckmann rearrangement); sigmatropic rearrangements

Metathesis and click chemistry: Definition, classes of reactions, catalysts used, mechanistic aspects and synthetic applications of methathesis reactions and click reactions in organic chemistry with suitable examples

Unit II

3. Ultraviolet and visible (UV-vis) spectroscopy: Application (3 lectures)

Recapitulation of the principle, preparation of samples for UV-vis spectroscopy, effects of solvents, chromophores and auxochromes, characteristic absorptions of varying chromophoric systems, applications

4. Infrared (IR) spectroscopy: Application (3 lectures)

Recapitulation of the principle, Fourier transform infrared spectroscopy (FTIR), preparation of samples for infrared spectroscopy, characteristic group frequencies and applications

5. Nuclear Magnetic Resonance (NMR) spectroscopy: General principles and application (10 lectures)

^{1}H-NMR spectroscopy: General introduction and definition; chemical shifts; spin-spin interaction; shielding mechanism; mechanism of measurement; chemical shifts and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohol, phenols, enols, carboxylic acids, amines, amides & mercapto); chemical exchange; effect of deuteration; complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling, stereochemistry; hindered rotation; Karplus curve-variation of coupling constant with dihedral angles; simplification of complex spectra - nuclear magnetic double resonance, shift reagents, solvent effect; Fourier transform technique; nuclear Overhauser effect (NOE); resonance of other nuclei, ^{19}F, ^{31}P, etc

Carbon-13 NMR spectroscopy - general considerations; chemical shift values (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon); coupling constant; Two Dimensional NMR Spectroscopy - COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.

6. Mass spectrometry: General principles and application (04 lectures)

Introduction; ion production - EI, CI, FD and FAB; factors affecting fragmentation; ion analysis; ion abundance; Mass spectral fragmentation of organic compounds; common functional groups; molecular ion peak; metastable peak; McLafferty rearrangement; nitrogen rule; high resolution mass spectrometry; examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

7. Combined spectral applications (05 lectures)

Applications of all the spectroscopic techniques (UV, FT-IR, NMR and Mass) in a combined manner to solve structural problems of unknown organic compounds

Suggested books

E. L. Eliel, S. H. Wilson and L. N. Mander,*Stereochemistry of Organic Compounds*, John Wiley & Sons, Inc., 2003.

E. L. Eliel, *Stereochemistry of Carbon Compounds*, Tata McGraw-Hill Edition, New Delhi, 1988.

D. Nasipuri, *Stereochemistry of Organic Compounds (Principles and Applications),* 2nd Edn, Wiley Eastern Limited, New Delhi, 1994.

E.L. Eliel, N.L. Allinger, S. J. Angyal and G.A Morrison, *Conformational Analysis*,John Wiley & Sons, Inc., 1967.

J. Eames and J. Peach, *Stereochemistry at a Glance*, Blackwell Science, 2003.

K. Mislow and W. A. Benjamin, *Introduction to Stereochemistry*New York, 1965.

B. Testa, *Principles of Organic Stereochemistry,*Marcel Dekker, New York, 1979.

E. Juaristi, *Stereochemistry & Conformational Analysis*,John Wiley & Sons, Inc., 1991.

M. Nogradi, *Stereochemistry: Concepts and Applications*, Pergamon Press, New York, 1981

Hua-Jie Zhu,*Organic Stereochemistry: Experimental and Computational Methods*, Wiley-VCH, 2015.

Michael B. Smith and Jerry March, *March's Advanced Organic Chemistry (Reactions, Mechanisms, and Structure),* 5th Edn., John Wiley & Sons, Inc., 2001.

Reinhard Bruckner, *Advanced Organic Chemistry (Reaction Mechanisms)*, Harcourt/Academic Press, 2002.

Thomas H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry.*3rd Edn., Addison-Wesley, 1998.

Peter Sykes, *A Guidebook to Mechanism in Organic Chemistry*, 6thEdn., Orient Longman Ltd., 1970.

Lloyd N. Ferguson, *The Modern Structural Theory of Organic Chemistry*, Prentice-Hall of India Pvt. Ltd., New Delhi, 1963.

R. H. Grubbs and D. J. O'leary (Eds), *Handbook of Metathesis* – vol. 1 and 2, Wiley-VCH, 2015.

D. L. Pavia, G. M. Lampman and G.S. Kriz, *Introduction to Spectroscopy*, 3^{rd}Edn.,Harcourt, Inc., 2001.

R. M. Silverstein, G. C. Bassler and T. C. Morrill, *Spectroscopic Identification of Organic Compounds*, 5^{th} Edn., John Wiley & Sons, Inc., 1991.

D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 5^{th} Edn., Tata McGraw-Hill Edition, New Delhi, 2004.

William Kemp, *Organic Spectroscopy*, 3^{rd}Edn.,Macmillan Press Ltd., 1991.

G. Siuzdak, *Mass Spectrometry for Biotechnology*, Academic Press, 2005.

H. Budzikiewicz, C. Djerassi and D. H. Williams, *Interpretation of Mass Spectra of Organic Compounds*, Holden-Day Inc., 1965.

J. S. Splitter and F. Tureček,*Applications of Mass Spectrometry to Organic Stereochemistry*, Wiley-VCH, 1994.

Atta-ur-Rahman and Md. Iqbal Choudhary, *Solving Problems with NMR Spectroscopy*, Academic Press, Inc., 1996.

Jag Mohan, *Organic Spectroscopy (Principles and Chemical* Applications), 2^{nd}Edn.,Narosa Publishing House Pvt. Ltd., New Delhi, 2004.

Norman S. Bhacca and D. H. Williams, *Applications of NMR Spectroscopy in Organic Chemistry*, Holden-Day, Inc., 1964.

L. M. Jackman and S. Sternhell, *Applications of Nuclear Magnetic Resonance Spectroscopy In Organic* Chemistry, 2^{nd} Edn., Pergamon Press, Oxford. Second Edition. 1969.

R. G. Linington, P. G. Williams and J. B. MacMillan, *Problems in Organic Structure Determination: A practical Approach to NMR Spectroscopy,* CRC Press, Taylor & Francis Group, 2016.

MSCCHEMC103: Physical Chemistry General I

Course objectives: To understand the basic aspects of classical physics and their drawbacks. Necessity of introduction of quantum mechanics to explain the drawbacks of classical physics. Understanding of wave – particle duality model. How uncertaintity appears in electron space. Understanding of the various kinds of motion (translation, rotation and vibration) of a particle.

Learning outcomes: After completing the course the student will be expected to be able to: Differentiate the basic principles, assumptions of classical and quantum chemistry and their consequences; understand that electron has both wave and particle nature; explain the varioous aspects of translational, rotational and vibrational motion using quantum approach.

Unit I

1. Quantum mechanics I (13 lectures)

Drawback of classical physics: A brief discussion on Black Body radiation, photo-electric effect and Double slit experiment .Wave-particle duality. Uncertainty principle, Operators in QM, Operator algebra, Commutation relation, Eigen functions and Eigen values, Postulates of QM, Ehrenfest's theorem, Schrodinger Equations, Theorems of QM. Few Model Systems, their solutions: Particle in 1-d Box, Selection Rules. Discussion on Bohr’s correspondence principle. Checking the validity of Schrodinger wave equation based on correspondence principle and Heisenberg’s Uncertainty principle Particle in 3-d Box, Particle in a ring and in a sphere, Tunneling.

2. Atomic and molecular spectroscopy: principle and application (12 lectures)

Review of basic spectroscopy, Hydrogen energy levels, spectroscopic transitions and selection rules, Multi-electron Atoms, Vector model, orbital and spin angular momentum of electrons, normal and anomalous Zeeman and Paschenback effects, Stern-Gerlach experiment, LS and jj coupling, spin-orbit coupling, atomic energy terms and term symbols, hyperfine structure

Rotational spectra: diatomic molecules as rigid rotors - energy levels, selection rules and spectral features, isotope effect, intensity distribution, effect of non-rigidity on spectral features; vibrational spectra of diatomics: potential energy of an oscillator, Harmonic Oscillator approximation, energy levels and selection rules, anharmonicity and its effect on energy levels and spectral features: overtones and hot bands, vibration-rotation spectra of diatomics: origin; selection rules; P, Q and R branches; Raman spectra: origin, selection rules, classical and quantum treatment of rotational and vibrational Raman spectra of diatomics, resonance Raman spectroscopy; NMR spectra: theory, relaxation process, spin interactions - its origin, equivalent protons, qualitative idea of energy levels of AX, AX2 and AX3 systems, a few representative examples

Unit II

3. Solutions thermodynamics and electrochemistry (15 lectures)

Partial molar quantities, significance and the determination of partial molar quantities, Thermodynamics of ideal and non-ideal binary solutions, excess functions and their determination, Activity co-efficients, Experimental determination of activity coefficients of electrolytes and non-electrolytes, Ion-Ion interactions, Debye-Huckel theory, Limiting and extended Debye Huckel equations for activity coefficients, ion-solvent interaction: Born model and Born equation, enthalpy of ion-solvent interaction and its calculation, Eley-Evan model, solvation number and methods for determination of solvation number, ion association: Bjerrum equation, fraction of ions associated, ion association constant; electrode kinetics: relation between current and rate of electrode reaction, current-overpotential relationship, Tafel equation and its importance

4. **Statistical thermodynamics** (10 lectures)

Motivation for study, Entropy and Probability, Stirling approximations, Maxwell-Boltzmann Distribution, Gibbs paradox, Sackur-Tetrode equation, concept of partition functions, translational, rotational, vibrational and electronic partition functions, Thermodynamic properties in terms of partition functions, Equilibrium constant , Equipartition principle, Einstein theory of specific heat capacity of solids.

Suggested books

L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, New York, 1939.

H. Eyring, J. Walter and G. F. Kimball, *Quantum Chemistry*, Wiley, New York, 1944.

P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.

L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, New York, 1985.

A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi, 1989.

F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, New Delhi, 1990.

D. A. McQuarrie, *Quantum Chemistry*, Viva Books Pvt. Ltd, New Delhi, 2003.

I. N. Levine, Quantum Chemistry, PHI Learning Pvt. Ltd, New Delhi, 2010.

M. Jammer, Conceptual Development of Quantum Mechanics, McGraw-Hill, 1966.

E. Merzbacher, Quantum Mechanics, Wiley, 1998.

S. M. Blinder, Introduction to Quantum Mechanics, Elsevier Academic, 2004.

H. E. White, *Introduction to Atomic Spectra*, McGraw-Hill Kogakusha Ltd., Tokyo, 1934.

G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill International Book Company, Tokyo, 1982.

C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Edn, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1994.

J. D. Graybeal, *Molecular Spectroscopy*, McGraw-Hill International Editions, Spectroscopy series, 1998.

D. A. McQuarrie and J. D. Simon, *Molecular Thermodynamics*, University Science Books, California, 1999.

I. N. Levine, *Physical Chemistry*, Tata McGraw-Hill, New Delhi, 1978. K. Denbigh, *Principles of Chemical Equilibrium*, Cambridge University Press, Cambridge, 1981. I. M. Klotz and R. M. Rosenberg, *Chemical Thermodynamics*, John Wiley, New York, 1994.

G. W. Castellan, *Physical Chemistry*, 3rd Edn, Narosa Publishing House, 1995.

N. A. Gokcen and R. G. Reddy, *Thermodynamics*, Plenum Press, New York, 1996.

G. K. Vemulapalli, *Physical Chemistry*, Prentice-Hall, India, 1997.

P. W. Atkins, *Physical Chemistry*, Oxford University Press, Oxford, 1998.

R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, Oxford University Press, Oxford, 2000.

J. O'M. Bockris and A. K. N. Reddy, *Modern Electrochemistry*, Vol I, Plenum Press, New York, 1970.

MSCCHEMC104: Analytical Chemistry General I

Course Objective: To study the terminology and special notation of statistical analysis in analytical and nuclear measurements to minimize the error in a chemical system and to organize data into a regular or a grouped frequency distribution table, and understand data that are presented in a table. To learn and apply the basic principles and concept of different separation and purification techniques in order to separate, purify and identify compounds or a chemical species. To learn about the thermal stability of different materials using various thermal techniques like TGA, DTA, DSC, etc., along with the basic idea about different theories and their applications. To understand the different electrochemical concepts utilized in different analytical methods. Basic knowledge about three electrode system, overpotential, and different electrode probes. To learn the basic principles of different electroanalytical techniques such as voltametry, amperometry, etc.

Learning Outcome: At the end of this course learners should be able to calculate different analytical parameters and solve different problems and count different data of a chemical reaction. Learners should be able understand the solvent extraction, chromatographies techniques for purification and separation of compounds. They also able to familiar with different aspect of solvent extraction, chromatographies techniques and can apply their theoretical knowledge in practical field of work. The learners should be able to understand the thermal properties of different materials and can measure the thermal stability of materials. Can solve problems based on various thermal concepts, design experiments with improved sample preparation, measurement procedures and tools, quantify analytes with proper data handling and analysis, and calculate various thermodynamic parameters. The learners should be able to plot and explain different curves such as polarography, stripping voltametry, MDE etc for estimation of different metal ions and oxidation states in electrolytic mixture solution etc.

Unit I

1. Statistical methods in analytical methods (08 lectures)

Application of counting statistics in analytical and nuclear measurements: probability and binomial distribution, radioactivity as a statistical phenomenon, standard deviation of counting data, Poisson distribution, optimization of counting experiments

2. Separation techniques (17 lectures)

Preamble, successive extraction and separation; techniques of solvent extraction: Craig extraction and counter current distribution; ionic liquid assisted and supercritical solvent extraction, problems; chromatography: mathematical relations of capacity, selectivity factor, distribution constant and retention time; chromatogram, elution in column chromatography: band broadening and column efficiency; van Deemter equation; column resolution, numerical problems, gas chromatography, high performance chromatography and supercritical fluid chromatography: principles, methods, comparison and applications; size-exclusion chromatography, ion chromatography and capillary electrophoresis: principles, methods and applications

Unit II

3. Thermal methods (10 lectures)

Different methods of analysis: TGA, DTA, DSC; thermogram, applications, thermal stability of covalent and non-covalent bonds, thermal degradation, single crystal phase transformation, thermochemiluminescence, different types of titrations and their applications, solid state reaction kinetics

4. Elecroanlytical methods I (15 lectures)

Fundamentals, electrochemical cell, reference and indicator electrodes, supporting electrolyte, solvent, electrolytic process, three electrode system, DME, Ilkovic equation, Ilkovic-Heyrolsky equation, test of reversibility, current-voltage diagram, DC and AC polarography, Cottrell equation, stripping voltammetry, amperometric titration, membrane electrodes, electrode-solution interface layer, gas-sensing probe

Suggested books

D. A. Skoog, D. M. West and F. J. Holley, *Fundamentals in Analytical Chemistry*, 5th Edn, Saunders, Philadelphia, 1988.

G. D. Christian, *Analytical Chemistry,* 6th Edn, Wiley-India, New Delhi, 2004.

M. Koel and M. Kaljurand, *Green Analytical Chemistry,* RSC Publishing, Cambridge, 2010.

Y. Marcus and A. S. Kertes, *Ion Exchange and Solvent Extraction of Metal Complexes*, Wiley Interscience, New Jersey, 1969.

E. Heftman, *Chromatography*, Reinhold, New York, 1969.

H. F. Walton and W. Reiman, *Ion Exchange in Analytical Chemistry*, Pergamon Press, Oxford, 1970.

J. A. Dean, *Chemical Separation Methods,* Van Nostrand Reinhold, London, 1970.

D. G. Peters, J. M. Hayes and G. M. Hieftje, *Chemical Separations and Measurements: Theory and Practice of Analytical Chemistry*, Saunders, Wiley Interscience, New York, 1974.

A. Tarter,*Advanced Ion Chromatography*, Wiley Interscience, New York, 1989.

S. Lindsay and J. Barnes, *High Performance Liquid Chromatography*, John Wiley, New York, 1992.

G. D. Christian, *Analytical Chemistry*, 5th Edn, Wiley, New York, 1994.

S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, Wiley Eastern Ltd., New Delhi, 1998.

C. Duval, *Inorganic Thermogravimetric Analysis*, Elsevier Publishing Co, New York, 1963.

W. W. Wendlandt, *Thermal Methods of Analysis*, Interscience Publishers, New York, 1964.

R. C. McKenzie (Ed), *Differential Thermal Analysis*, Academic Press, New York, 1970.

D. R. Crow, *Polarography of Metal Complexes*, Academic Press, London, 1979.

A. J. Bard and L. F. Faulkner, *Electrochemical Methods – Fundamentals and Applications,* 2^{nd} Edn, Wiley, New York, 1998.

C. G. Zoski (Ed) *Handbook of Electrochemistry,* Elsevier, New York, 2007.

J. Goodisman, *Electrochemistry: Theoretical Foundations*, Wiley, New York, 1987.

R. J. Gale (Ed), *Spectroelectrochemistry: Theory and Practice*, Plenum Press, New York, 1988.

J. O’M. Bockris and S. U. M. Khan, *Surface Electrochemistry*, Plenum Press, New York, 1993.

C. M. A. Brett and A. M. O. Brett, *Electrochemistry: Principles, Methods and Applications,* Oxford University Press, Oxford, 1993.

K. V. Kordesch, *Fuel Cells and Their Applications*, VCH, Weinheim, 1994.

D. T. Sawyer, A. Sobkowiak and J. L. Roberts, Jr, *Experimental Electrochemistry for Chemists*, 2nd Edn, Wiley, New York, 1995.

P. G. Bruce, *Solid-state Electrochemistry*, Cambridge University Press, Cambridge, 1995.
W. Schmickler, *Interfacial Electrochemistry*, Oxford University Press, Oxford, 1996.
C. A. Vincent and B. Scrosati, *Modern Batteries*, 2nd Edn, Arnold, London, 1997.
C. H. Hamann, A. Hamnett and W. Vielstich, *Electrochemistry,* Wiley-VCH, Weinheim, Germany, 2007.

Practical Papers (For Each, Full Marks: 50; Credit: 4)

MSCCHEMC105: Inorganic Chemistry General: Practical

Course Objective: To explore the basic chemistry in aqueous medium, solubility product, color, texture, solubility, group chemistry etc. of some common inorganic salts (both cations and anions)

Learning outcome: Detect the cations and anions present in unknown inorganic sample.

Content:

1. Preparation/synthesis of inorganic and coordination compounds: selected simple salts, double salts and coordination compounds with some common inorganic and organic ligands
2. Characterization using microanalysis, conductivity measurement and spectroscopic analysis

MSCCHEMC106: Organic Chemistry General: Practical

Course Objectives: The learners should be able to: Detection and identification of organic compounds qualitatively.

Learning Outcomes: At the end of the course, the learners should be able to: Identify different organic compounds both solid and liquid samples. Determine the m.p., b.p. solubility.

Content:

1. Separation (chemical/column chromatographic) of binary mixtures of solid-solid/liquid-solid/liquid-liquid organic samples and identification of individual components
2. Synthesis of organic compounds involving important chemical reactions (halogenations, nitration, diazotisation, Beckmann transformation, photochemical reaction, Sandmayer reaction, pinacol-pinacolone rearrangement, etc.)

Semester-II

Theoretical Papers (For Each, Full Marks: 50; Credit: 4)

MSCCHEMC201: Inorganic Chemistry General II

Course Objective lanthanoids and Actinoids are chemical elements that are present in lanthanide and actinide series of the periodic table respectively. These elements are known as f block elements. This is because their valence electrons are in the f orbital of their atoms. They are also called inner transition metals. Electronic spectra and magnetic properties of these element are also discussed. Able to interpret the EPR plots, hyperfine splitting etc. Differential UPS, UV PES, AUGER and XRF.

Learning Outcome Student should learn the synthesis, structures, bonding and reactivity of lanthanoids and actinides element. Industrial application as well as medicinal importance of these compounds will also be discussed. Fluxionality, distortion and dynamic equilibria; EPR: anisotropy, intensity, hyperfine splitting, photoelectron spectroscopy, XPS, UPS, AUGER, XRF.

Unit I

1. Chemistry of elements and their compounds (25 lectures)

Elements – structural versatility coupled with properties; compounds – design and benign synthesis, isolation, characterization, solution structure, molecular aggregate, crystalline architecture, spectral, magnetic and catalytic properties and application in chemistry, biology and materials science

Non-transition and transition metal ion homoleptic/heteroleptic and homonuclear/heteronuclear complexes of different dimensions with varied mono- and polydentate blockers containing carbon, nitrogen, phosphorus, chalcogen, halogen donors with/without mono-/polydentate pure/mixed bridges and counter ions

Mono- and polynuclear compounds of lanthanoid and actinoid ions stressing on choice of different multidentate chelators and congregators with special emphasis on electric, magnetic, conducting, superconducting and fluorophoric behaviours

Unit II

2. Inorganic reaction mechanism I (13 lectures)

Preamble, factors affecting the rate of a chemical reaction, analysis of rate data, complex rate laws, kinetically indistinguishable schemes, nucleophilicity and rate scales: Edward scale, n_{Pt} scale, Gutmann donor number, Drago E & C scale, trans- and cis- effects, water exchange rates, proton ambiguity, mechanistic simulation; associative, dissociative, interchange, nucleophilic, electrophilic, insertion pathways; Hammett relation, application of LFER in chemical kinetics

3. Cluster compounds (12 lectures)

Classification, elemental clusters, cluster skeletal electron (Elm) counting, higher boron hydrides-structures and reactions, equation of balance, Lipscomb topological diagrams, polyhedral skeletal electron pair theory (PSEPT), carboranes, metalloboranes and heteroboranes, metallocarboranes, zintl ions, chevrel compounds, infinite metal chains, multidecker molecules, cluster-surface analogy

Suggested books

J. D. Lee, *Concise Inorganic Chemistry*, Chapman and Hall, London, 1991.

N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, 2nd Edn, Pergamon, New York, 1997.

F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6^{th} Edn, John Wiley & Sons, Inc, New York, 1999.

G. Wulfsberg, *Inorganic Chemistry*, Viva Books Pvt. Ltd, New Delhi, 2001.

B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Edn, John Wiley & Sons, Inc, New York, 2001.

P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Shriver & Atkins Inorganic Chemistry*, 4th Edn, Oxford, 2006.

J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorgnic Chemistry: Principles of Structures and Reactivity,* 4th Edn, Pearson, New Delhi, 2006.

R. Xu, W. Pang and Q. Huo (Eds), *Modern Inorganic Synthetic Chemistry*, Elsevier, New York, 2011.

J. Crowe, T. Bradshaw and P. Monk, *Chemistry of Biosciences*, Oxford University Press, Oxford, 2006.

G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3rd Edn, Pearson, New Delhi, 2009.

J. R. Anderson and M. Boudart (Eds), *Catalysis: Science and Technology,* Springer, London, 2012.

G. Cao, *Nanostructures & Nanomaterials, Synthesis, Properties & Applications*, Imperial College Press, London, 2004.

L. Cademartiri and G. A. Ozin, *Concepts of Nanochemistry*, Wiley-VCH, Weinheim, 2009.

A. von Zelewsky, *Stereochemistry of Coordination Compounds*, Wiley, New York, 1996.

S. P. Sinha, *Systematics and Properties of Lanthanides*, Riedel, Dordrecht, 1983.

J. J. Katz, G. T. Seaborg and L. R. Morss (Eds), *The Chemistry of the Actinide Elements*, Vols I and II, 2nd Edn, Chapman and Hall, London, 1986.

J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, 2nd Edn, John Wiley and Sons, New York, 2009.

I. Pelant and J. Valenta, *Luminescence Spectroscopy of Semiconductors, Oxford,* New York, 2012.

J. O. Edwards and W. A. Benjamin, *Inorganic Reactions Mechanism*, INC, New York, 1965.

C. H. Langford and H. B. Gray, *Ligand Substitution Processes*, W. A. Benjamin, New York, 1966.

F. Basolo and R. G. Pearson, *Mechanism of Inorganic Reactions*, 2nd Edn, Wiley, New York, 1967.

D. Katakis and G. Gordon, *Mechanisms of Inorganic Reactions*, John Wiley & Sons, New York, 1987.

R. G. Wilkinns, *Kinetics and Mechanism of Reactions of Transition Metal Complexes*, 2nd Edn, VCH, Weinheim, 1991.

R. B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems*, Oxford University Press, Oxford, 1998.

J. D. Atwood, *Inorganic and Organometallic Reaction Mechanisms,* 2nd Edn, Wiley-VCH, Weinheim, 1997.

M. B. Wright, *Fundamental Chemical Kinetics – An Explanatory Introduction to the Concepts*, Harwood Publishing, Chichester, 1999.

S. Asperger, *Chemical Kinetics and Inorganic Reaction Mechanisms,* 2nd Edn, Springer, London, 2012.

C. E. Housecroft, *Cluster Molecules of the p-Block Elements,* Oxford University Press, Cambridge, 1994.

M. H. Chisholm (Ed), *Early Transition Metal Clusters with π-Donor Ligands,* VCH, New York, 1995.

D. M. P. Mingos (Ed.), *Structural and Electronic Paradigms in Cluster Chemistry*, Springer, Berlin, 1997.

P. Braunstein, L. A. Oro and P. R. Raithby (Eds), *Metal Clusters in Chemistry*, Wiley-VCH, Weinheim, 1999.

M. Driess and H. Noth (Eds), *Molecular Clusters of the Main Group Elements,* Wiley-VCH, Weinheim, 2004.

T. P. Fehlner, J. -F. Halet and J. -Y. Saillard, *Molecular Clusters - A Bridge to Solid State Chemistry*, Cambridge University Press, Cambridge, 2007.

C. E. Housecraft and A. G. Sharpe, *Inorganic Chemistry*, 3rd Edn, Pearson Education Ltd, Essex, England, 2008.

MSCCHEMC202: Organic Chemistry General II

Course Objectives: The learners should be able to synthesis , reactivity & uses of various intermediates & their derivatives.

Learning Outcomes: At the end of the course, the learners should be able to: **Identify** the structure of various heterocycles & their derivatives. To know the importance, applications and uses of heterocyclic compounds.

Unit I

1. Organic name reactions (10 lectures)

Baeyer-Villiger oxidation; Barton reaction; Beckmann rearrangement; Birch reduction; Claisen rearrangement; Favorskii reaction; Fries rearrangement; Heck reaction; Mannich reaction; McMurry reaction; Michael addition; Perkin reaction; Sharpless asymmetric epoxidation; Stile coupling; Strecker reaction; Suzuki coupling; Wittig reaction; Yamaguchi esterification

2. Reaction intermediates (09 lectures)

Generation, stability & structure, and reactivity of the reaction intermediates, *viz.* carbocations, carbanions, carbon free-radicals, carbenes, benzynes and nitrenes

3. Synthetic polymers and biopolymers (06 lectures)

Introduction to polymers - synthetic polymers;principles of macromolecular synthesis: step-growth vs. chain-growth polymerizations; Dendrimers: Dendritic polymers and their potential applications; chemistry of biopolymers (carbohydrates, proteins, and nucleic acids)

Unit II

4. Chemistry of natural products: Chemistry and function (15 lectures)

Chemistry and function of some major groups of natural products such as terpenoids (*monoterpenoids*: geraniol, alpha-pinene, camphor, menthol, carvone; *sesquiterpenoids*: farnesol, zingiberine, caryophyllene, santonin; *diterpenoids*: abietic acid, taxol; *triterpenoids*: beta-amyrene, oleanolic acid, ursolic acid), alkaloids (papaverine, emitene, morphine, quinine, nicotine, ephedrine) andcarbohydrates (monosaccharides and disaccharides); concepts on biosynthetic pathways (*mevalonic acid*, *geranyl pyrophosphate*, *shikimic acid*) for natural products

5. Medicinal chemistry (10 lectures)

Concept of drug design (physiochemical principles and basis of drug design, quantitative description, physicochemical approach of drug molecules, different methods of drug design, Free Wilson method and its application to extrathermodynamic approach);pharmacodynamic and pharmacokinetic (drug absorption, distribution, metabolism and excretion) aspects;drug targets (enzymes, receptors, nucleic acids); membranes and receptors (drug transport mechanism and absorption processes, prodrugs and bioactivation, receptor theories and receptor models, drug receptor interactions); concept on lead compounds and lead modifications; pharmacophore; structure-activity relationship (SAR); clinical trials; bioavailability; computer-aided drug design(*de novo* design), docking procedures and molecular modeling; discussion with suitable examples of choice.

Suggested books

A. Hassner, I. Namboothiri, *Organic Syntheses Based on Name Reactions*, 3rd Edn., Elsevier, 2012.

B. P. Mundy and M. G. Ellerd,*Name Reactions and Reagents in Organic Synthesis*, John Wiley & Sons, 1988.

L. Kürti and B. Czakó, *Strategic Applications of Named Reactions in Organic Synthesis: Background and Detailed Mechanisms*, Elsevier Academic Press, 2005.

Z. Wang, *Comprehensive Organic Name Reactions and Reagents,* Wiley-VCH, 2009.

J. J. Li, *Name Reactions: A Collection of Detailed Reaction Mechanisms*, Springer, 2014.

G. Brahmachari, *Organic Name Reactions: A Unified Approach*, Narosa Publishing House Pvt. Ltd., New Delhi, 2012.

Michael B. Smith and Jerry March, *March's Advanced Organic Chemistry (Reactions, Mechanisms, and Structure),* 5th Edn, John Wiley & Sons, Inc., 2001.

Reinhard Bruckner, *Advanced Organic Chemistry (Reaction Mechanisms)*, Harcourt/Academic Press, 2002.

Reinhard Bruckner, *Advanced Organic Chemistry (Reaction Mechanisms)*, Harcourt/Academic Press, 2002.

J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, 2001.

F. A. Carry and R. J. Sundberg, *Advanced Organic Chemistry – Part-A and B,* 5th Edn, Springer, 2007.

L. G. Wade, Jr. and M. S. Singh, *Organic Chemistry*, 6th Edn, Pearson Education, 2008.

T. G. Graham and C. B. Fryhle, *Organic Chemistry*, 8th Edn, John Wiley & Sons, 2004.

C. J. Moody, *Reactive Intermediates*, Oxford University Press, 1992.

R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, *Organic Chemistry*, 7th Edn, Pearson Education, 2013.

S. Ebnesajjad, *Handbook of Biopolymers and Biodegradable Plastics: Properties, Processing and Applications,* PDL handbook series, William Andrew, 2013.

A. Walton, *Biopolymers*, Elsevier, 2012.

D. Plackett, *Biopolymers - New Materials for Sustainable Films and Coatings*, John Wiley & Sons, 2011.

P.J. Flory, *Principles of Polymer Chemistry*, Cornell University Press, 1953

M.M. Coleman and P.C. Painter, *Fundamentals of Polymer Science – An Introductory Text*, CRC Press, Taylor & Francis, 1998.

M.P. Stevens, *Polymer Chemistry: An Introduction*, Oxford University Press, 1998.

J.N. Nicholson, *The Chemistry of Polymers*, Royal Society of Chemistry, 2012.

D. A. Tomalia, J. B. Christensen and U. Boas, *Dendrimers, Dendrons and Dendritic Polymers: Discovery, Applications and the Future,* Cambridge University Press, 2012.

S. R. Sharma, *Biomolecules*, Discovery Publishing House, 2003.

R. J. Simmonds,*Chemistry of Biomolecules: An Introduction 1st Edition*, Royal Society of Chemistry, 2002.

D. Feldman and A. Barbalata, *Synthetic Polymers: Technology, Properties and Applications,* Springer, 1996.

G. Brahmachari, *Bioactive Natural Products*: *Chemistry & Biology*, Wiley-VCH, 2015.

S. K. Talapatra and B. Talapatra, *Chemistry of Plant Natural Products*, Springer, 2012.

T. Ogura, *Dynamic Aspects of Natural Products Chemistry*, CRC Press, 1997.

A. E. Osbourn and Lanzotti, V., *Plant-derived Natural Products: Synthesis, Function, and Application,* Springer, 2009.

J. R. Hanson, *Natural Products: The Secondary Metabolites*, Royal Society of Chemistry, 2003.

S. Hanessian,*Natural Products in Medicinal Chemistry: Methods and Principles in Medicinal Chemistry*, Wiley-VCH, 2014.

G. Brahmachari, *Handbook of Pharmaceutical Natural products – Vols. 1 and 2*, Wiley-VCH, 2010.
G. Brahmachari, *Chemistry and Pharmacology of Naturally Occurring Bioactive Compounds*, CRC Press, Taylor & Francis, 2013.
G. Brahmachari, *Bioactive Natural Products: Opportunities and Challenges in Medicinal Chemistry*, World Scientific Publishing Co., 2011.
S. V. Bhat, B. A. Nagasampagi and M. Sivakumar, *Chemistry of Natural Products*, Narosa Publishing House, New Delhi, 2005.
X. -T. Liang and W. -S. Fang, *Medicinal Chemistry of Bioactive Natural Products*, John Wiley & Sons, 2006.
P. Manitto, *Biosynthesis of Natural Products*, Ellis Horwood Ltd., 1981.
G. L. Patrik, An Introduction to Medicinal Chemistry, 3rd Edn, Oxford University Press, 2006.
C. G. Wermuth (Ed), The Practice of Medicinal Chemistry, Academic Press, Noida, India, 2008.
G. Thomas, *Fundamentals of Medicinal Chemistry*, 5th Edn, Oxford University Press, 2013.
R. B. Silverman, *The Organic Chemistry of Drug Design and Drug Action*,3rd Edn, Academic Press, 2014.
M. P. S. Ishar and A Faruk, *Syntheses of Organic Medicinal Compounds*, Alpha Science, 2006.
D. R. Budman,A. H. Calvert and E. K. Rowinsky, *Handbook of Anticancer Drug Development*, Lippincott Williams & Wilkins, Philadelphia, PA, USA, 2003.
E. Garrett-Meyer, *Principles of Anticancer Drug Development*, Springer, 2010.

MSCCHEMC203: Physical Chemistry General II

Course Objective: Symmetry in molecules can be used to predict several properties of molecules. The mathematical tool required for utilising symmetry is Group Theory. Different types of molecular property can be explained using basic principles of Group Theory. Construction of Group Multiplication Table, Character Table explores these things. This chapter consists of the basic principles of group theory. The Great Orthogonality Theorem (GOT) & its important corollaries are the main important part of the chapter. In this segment of group theory, procedure for construction of character tables for Abelian, Cyclic & Direct product groups have been explained by utilising the corollaries of GOT. Several applications of vanishing integral rule have been demonstrated. Actually this chapter is the gateway to the next chapter ―Group Theory III/Applications of Group Theory.

This chapter essentially deals with a major part of exactly solvable quantum mechanical problems. The analytical solutions of these problems involves the learning of some major mathematical techniques (e.g. Dirac's number operator formalism) frequently used in other parts of theoretical chemistry. A significant part of this chapter devoted to understand quantum numbers, orbital and spin angular momenta of electrons and space quantization.

Learning Outcome: In this chapter, at first, we have tried to give a lesson regarding the symmetry operation and symmetry multiplication table then the construction of Group Multiplication Table that can be used to predict the conjugate classes present within a given point group. Identification of point group is the main topic of this chapter. Similarity transformation and invariance of character under similarity transformation are two another important topics. The chapter ended with the knowledge of construction of character table of molecules belonging to different kinds of point group

It has been found that construction of character tables is one of the most important questions that have been asked in several entrance examinations like NET, GATE, TIFR etc. This chapter is also aimed at building up the underlying basic concepts of various chemical ideas used in theoretical as well as in experimental chemistry. After completing the course the student will be expected to be able to:

• explain and use the central concepts, theoretical descriptions, and fundamental approximations applied to atoms.

• treat the quantum mechanical formalism for identical particles and apply these to the structure of atoms.

• describe, carry out, and evaluate the various spectroscopic methods used to study atoms.

Thus the instructor thinks that this chapter has huge applicability in future research aspect. Students also get considerable amount of questions in various competitive examinations like GET/NET/ SET etc. from this chapter.

Unit I

1. Symmetry and group theory (25 lectures)

Concept of symmetry, symmetry elements and symmetry operations, optical activity, concept of groups, point symmetry groups, class, group multiplication tables, matrix representation, equivalent and reducible representations, irreducible representations, great orthogonality theorems statement and interpretation, proof of its corollaries, character table and its construction, number of times an irreducible representation occurs in a reducible one; the reduction of reducible representations, notation of irreducible representations, link between group theory and quantum mechanics, direct product representations, vanishing integrals and projection operators

Unit II

2. Quantum mechanics II (15 lectures)

Harmonic Oscillator: solution of Schrodinger equation of a harmonic oscillator using the operator method as well as the technique for solution of differential equation, selection rules for harmonic oscillator, checking the validity of Schrodinger wave equation based on correspondence principle, Heisenberg's Uncertainty principle, QM of rotational motion; angular momentum operators and their commutation relations, operator algebra and Ladder operators for rotational motion, solution of Schrodinger equation using the operator method as well as the technique for solution of differential equation, quantum mechanics of rigid rotor and its application

Hydrogen atom: Separation of translational and internal motion of a two-body problem, determination of radial part of the wave function, relation among principal, azimuthal and magnetic quantum number, nodal properties of angular part as well as the radial part of the hydrogen atom wave function, shape of the orbitals, space quantization, selection rules for hydrogen atom.

3. Chemical Kinetics (10 lectures)

Transition state theory, potential energy surfaces, concept of imaginary frequency, thermodynamic treatment of reaction rates, energy of activation, volume of activation, reactions in solutions, diffusion and activation controlled reactions, influence of solvent dielectric constant and ionic strength on reaction rates, linear free energy relationship, effect of substituents, Hammett's and Taft's constants, Hammet's acidity functions, Oscillatory reactions

Suggested books

S. C. Rakshit, *Molecular Symmetry Group and Chemistry*, The New Book Stall, Kolkata, 1988.

V. Heine, *Group Theory in Quantum Mechanics: An Introduction to Its Present Usage*, Dover Publication, New York, 1991.

D. M. Bishop, *Group Theory and Chemistry*, Oxford University Press, Oxford, 1993.

A. Vincent, *Molecular Symmetry and Group Theory*, John Wiley & Sons, New York, 1998.

F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn, John Wiley & Sons, New York, 1999.

L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, New York, 1939.

H. Eyring, J. Walter and G. F. Kimball, *Quantum Chemistry*, Wiley, New York, 1944.

P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.

L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, New York, 1985.

A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi, 1989.

F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, New Delhi, 1990.

D. A. McQuarrie, *Quantum Chemistry*, Viva Books Pvt Ltd, New Delhi, 2003.

I. N. Levine, Quantum Chemistry, PHI Learning Pvt. Ltd, New Delhi, 2010.

M. Jammer, Conceptual Development of Quantum Mechanics, McGraw-Hill, 1966.

E. Merzbacher, Quantum Mechanics, Wiley, 1998.

S. M. Blinder, Introduction to Quantum Mechanics, Elsevier Academic, 2004.

K. J. Laidler, *Reaction Kinetics*, Vols I and II, Pergamon Press, London, 1970.

L. P. Hammett, *Physical Organic Chemistry*, McGraw-Hill Book Company, New Delhi, 1970.

J. Albery, *Electrode Kinetics*, Oxford Chemistry Series, Clarendron Press, Oxford, 1975.

K. J. Laidler, *Chemical Kinetics*, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1988.

M. R. Wright, *Fundamental Chemical Kinetics*, Horwood Publishing, 1999.

MSCCHEMC204: Analytical Chemistry General II

Course Objective: To understand the composition of the nuclear structure, its stability and properties, different nuclear reactions and radioactive equilibrium and basic principles of Mossbauer spectroscopy and induce the students to take up nuclear research in their higher studies. Environmental chemistry helps us to prevent hazards from industry and encourage to design environment friendly chemical methods and to develop green alternative chemical reactions.

Course Outcome: Understand composition of the nuclear structure, its stability and properties, different nuclear reactions and radioactive equilibrium. Evaluate different nuclear configuration of different isotopes. Able to measure magnetic moments and quadrupole moments. Explain the Mossbauer spectra. Identify and define various types of nuclear changes or processes including fission, fusion and decay reactions. Understand the concept of rate of change and half-life in the context of nuclear decay. Able to develop green methods for synthesis. Familiar with different adverse effect of chemical industry on environmental.

Unit I

1. Nuclear force, structures and properties (18 lectures)

Fundamentals, nuclear composition, different nuclear forces; concept of nuclear angular momentum, magnetic dipole moment and electronic quadruple moment (elementary idea), nuclear magnetic dipole moment and electric quadruple moment in terms of shell model, parity of nuclear energy states; liquid drop model, formulation of semi-empirical binding energy equation, mass parabola and application of binding energy equation; nuclear reactions, Q-value and cross section of nuclear reaction, compound nucleus theory, shell model, nuclear magic number and its derivation from nuclear potential well, calculation of nuclear spin, nuclear isomerism and non-optical transitions; two body problem - properties of deuteron and derivation of depth-range relationship, its applications in explaining nature of nuclear force, nuclear models - strong and weak interaction, collective model, Fermi gas model, nuclear excitation, idea of nuclear temperature and entropy

2. Nuclear quadruple resonance and Mossbauer spectroscopy (07 lectures)

NQR, Mossbauer effect - conditions, nuclear recoil, Doppler effect, instrumentation, chemical shift examples, quadrupole effect, effect of magnetic field, effect of simultaneous electric and magnetic fields, typical spectra of iron and tin compounds

Unit II

3. Theory of radioactive decay and radioactive equilibrium (10 lectures)

Introduction, quantum mechanical aspects of radioactive disintegration, alpha decay paradox and its explanation in terms of tunnel effect, Geiger-Muller relationship, time-dependant perturbation theory, Golden rule and its application in explaining beta and gamma transition, selection rules

Successive disintegration, Bateman equation, secular and transient equilibrium, no equilibrium; analysis of special types of successive disintegration, formation of radioelement in a nuclear reaction, activation analysis

4. Surfactants and utility (07 lectures)

Preamble, surface excess; classification of surfactants BET isotherm, LB film, membrane equilibrium, micellaisation,Kraft temperature, synthetic application of micellar catalysis, mixed micelles, foaming of surfactant solution, different types of interface, emulsion and emulsifier, photochemistry and redox reaction in micellar systems, nanoemulsion and stabilisation

5. Environmental chemistry (08 lectures)

Sustainable development, twelve principles of green chemistry and implementations, atom economy, environmental E-factor, role of catalysts, microwave and ultrasound irradiation in green synthesis, traditional and alternative commercial syntheses of ibuprofen, adipic acid and maleic acid etc, green chemistry in action developing foam, whitening agent, detergent builders, green insecticides, biosynthesis of synthetic chemical, photochemical reactions in atmosphere, photochemical smog and stratospheric ozone depletion; chemicals from renewable feedstock

Suggested books

B. Harvey, *Introduction to Nuclear Physics and Chemistry*, Prentice Hall, New York, 1965.

S. Glasstone, *Source Book of Atomic Energy*, East-West Press Private Ltd, New Delhi, 1967.

R. D. Evans, *The Atomic Nucleus*, McGraw-Hill, New York, 1979.

G. R. Choppin and J. Rydberg, *Nuclear Chemistry: Theory and Applications,* Pergamon Press, Oxford, 1980.

G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller, *Nuclear and Radiochemistry*, 3rd Edn, Jhon Wiley & Sons Inc, New York, 1981.

H. J. Arnikar, *Essentials of Nuclear Chemistry*, 4th Edn, New Age International (P) Ltd Publications, New Delhi, 2001.

D. D. Sood, A.V. R Reddy and N. Ramamoorty, *Fundumentals of Radiochemistry*, Yancas, Mumbai, 2004.

W. D. Loveland, D. J. Morrissey and G. T. Seaborg, *Modern Nuclear Chemistry*, Wiley Interscience, New Jersey, 2006.

V. I. Goldanskii and R. H. Herber, *Chemical Applications of Mossbauer Spectroscopoy*, Academic Press, New York, 1968.

N. N. Greenwood and T. C. Gibb, *Mossbauer Spectroscopy*, Chapman and Hall, London, 1971.

R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.

J. M. Hollas, *Modern Spectroscopy*, Wiley, New York, 1996.

D. D. Clayton, *Principles of Steller Evolution and Nucleosynthesis,* Chicago University Press, Chicago, 1983.

K. Heyde, *Basic Ideas and Concepts in Nuclear Physics,* IOP, Briston, 1999.

G. R. Choppin, J. O. Liljenjin and J. Rydberg, *Radiochemistry and Nuclear Chemistry,* Butterworth-Heinmann, Woburu, 2002.

Y.Moroi, *Micelles, Theoretical and Applied Aspects,* Plenum Press, New York, 1992.

M. M. Rieger and L. D. Rheis (Eds), *Surfactants in Cosmetics,* Marcel Dekker Inc, New York, 1997.

K. Holmberg, B. Jonsson, B. Kronberg and B. Lindman, *Surfactants and Polymers in Aqueous Solution,* John Wiley & Sons, New York, 2002.

M. N. Khan, *Miceller Catalysis,* Taylor and Francis Group, New York, 2007.

T. F. Tadros (Ed), *Emulstion Science and Technology,* Willey-VCH, Verlag GmbH and Co, 2009.

O. Hutzinger (Ed), *The Handbook of Environmental Chemistry*, Springer-Verlag, Weinheim, 1980.

D. F. S. Natusch and P. K. Hopke, *Analytical Aspects of Environmental Chemistry*, John Wiley & Sons, New York, 1983.

R. M. Harrison (Ed), *Pollution: Causes, Effects and Control*, Royal Society of Chemistry, Great Britain, 1990.

J. E. Fergusson, *The Heavy Elements: Chemistry, Environmental Impact and Health Effects*, Pergamon Press, Oxford, 1990.

S. E. Manahan, *Environmental Chemistry*, Lewis Publishers, Boston, 1991.

R.Sanghi and V. Singh, *Green Chemistry for environmental remediation*, Wiley, New York, 2012.

Practical Papers (For Each, Full Marks: 50; Credit: 4)

MSCCHEMC205: Physical Chemistry General: Practical

Course objectives:

- To validate the conceptual understanding acquired from the theory classes.

- To perform experiments applying concepts of conductivity / EMF of ions in solution, chemical kinetics, equilibrium, etc.
- To perform the data processing acquired from the experiments using numerical or computational method like plotting in origin etc.

Learning Outcomes: At the end of the course, the learners should be able to:

• explain the principle behind the experiments performed in the laboratory

• plan and perform experiments and interpret experimental results.

• process data, plot experimental data and thereby interpret the experimental results.

Course Content:

1. Experiments in equilibrium and kinetics

3. Instrumental methods: colorimetry polarimetry, conductometry and potentiometry

4. Data processing and elementary numerical techniques

MSCCHEMC206: Analytical Chemistry General: Practical

Course Objective: To learn methods for estimating and analyzing different metals present in different ores and alloys. Applications of different separation techniques learned in theory classes.

Learning Outcome: Able to identify the metals present in different ores and alloys. Able to separate, purify and identify different compounds from a mixture. Able to use UV-Vis spectrophotometer and can verify Beer's law by spectrophotometric study.

Course Content:

1. Experiments on quantitative estimation: analysis of selected ores and alloys
2. Separation techniques involving ion-exchange and solvent extraction
3. Titrimetric estimation of different organic compounds
4. Beer's law: application in different chemical matrices

Extra Departmental Electives (Full Marks: 50; Credit: 4)

MSCCHEMMIE201: Supramolecular and Medicinal Chemistry

Course Objective: To impart knowledge of different types of supramolecules, structures and their applications as organic-inorganic materials, sensors, and devices. In particular, supramolecular chemistry is focused on understanding the physics of noncovalent bonding. Teaches the chemistry/mechanism of action of various commercially available antibiotics and life saving drugs

Outcome: The students will acquire knowledge of (i) details of synthesis, structure as well as reaction of supramolecules, (ii) Molecular recognition and nature of bindings involved in biological systems (iii) Structure of supramolecules of various types in solid state (iv) Applications of supramolecules in miniaturization of molecular devices.

Course Content:

Concept and language, choice of building blocks – a sheer necessity, atomic and molecular valences, supramolecular orbitals, principle of three C's, pallet of non-covalent forces such as hydrogen bond, π…π, C-H…π, halogen…π, S…π, cation…π, hydrophobic, hydrophilic etc interactions and their harnessing towards crystal engineering, structure directed supramolecular arrays, allosterism, proton and hydride sponges, lock and key principle, host-guest interaction, self organization and self complementarity, superstructures in organic, inorganic, metallo-organic and organometallic compounds, 0D, 1D, 2D, 3D architectures and hierarchies, crystal synthesis, supramolecular devices, deliberate isolation of different functional materials,molecular receptor and specific molecular recognition

Drug discovery and history of medicinal chemistry, drug and medicine, physiochemical principles and basis of drug design, pharmacodynamic and pharmacokinetic (drug administration, dosing, absorption, distribution, metabolism and excretion) aspects; drug targets (enzymes, receptors, nucleic acids); prodrugs and bioactivation, concept on lead compounds and lead modifications; pharmacophore; structure-activity relationship, clinical trials; bioavailability; computer-aided drug design; uses of different drugs and medicines: carcinogenesis, applications of chelators and metal chelates of different generations; antitumour, anticancer and anti-AIDS drugs, mechanistic pathway, limitation, future dimension

Suggested books

F. Vogtle, *Supramolecular Chemistry: An Introduction*, Wiley, Chichester, 1991.

B. Dietrich, P. Viout and J. -M. Lehn, *Macrocyclic Chemistry – Aspects of Organic and Inorganic Supramolecular Chemistry*, VCH, Weinheim, 1993.

J. -M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, VCH, Weinheim, 1995.

G. A. Jeffrey, *An Introduction to Hydrogen Bonding,* Oxford University Press, Oxford, 1997.

S. T. Hyde, B. Ninham, S. Anderson, Z. Blum, T. Landh, K. Larsson and S. Liddin, *The Language of Shape,* Elsevier, Amsterdam, 1997.

G. R. Desiraju (Ed), *Crystal Design: Structure and Function, Perspectives in Supramolecular Chemistry*, Vol 7, Wiley, Chichester, 2003.

J. W. Steed and J. L. Atwood,*Supramolecular Chemistry,* 2nd Edn, John Wiley & Sons, New York, 2009.

K. Rurack and R. Martinez-Manez (Eds), *The Supramolecular Chemistry of Organic-Inorganic Hybrid Materials,* John Wiley & Sons, Hoboken, New Jersey, 2010.

E. R. T. Tiekink and J. Zukerman-Schpector (Eds), *The Importance of Pi-Interactions in Crystal Engineering: Frontiers in Crystal Engineering,* 1st Edn, John Wiley & Sons, Chichester, UK, 2012.

G. L. Patrik, *An Introduction to Medicinal Chemistry*, 3rd Edn, Oxford University Press, 2006.

C. G. Wermuth (Ed), *The Practice of Medicinal Chemistry*, Academic Press, Noida, India, 2008.

X. -T. Liang and W. -S. Fang, *Medicinal Chemistry of Bioactive Natural Products*, John Wiley & Sons, 2006.

S. Sánchez and A. L. Demain, *Antibiotics: Current Innovations and Future Trends,*Caister Academic Press, 2015.

K. Chatterjee and E. J. Topol, *Cardiac Drugs*, 1st Edn, Jaypee Brothers Medical Pub., 2013.

W. H. Frishman and D. A. Sica, *Cardiovascular Pharmacotherapeutics,* 3rd Edn, CardioText, 2011.

Atta-ur-Rahman and M. I. Choudhary, *Frontiers in Cardiovascular Drug Discovery*, Bentham Publications, 2010.

S. Quideau, *Chemistry and Biology of Ellagitannins*, World Scientific Publishing Co., 2009.

X. -T. Liang and W. -S. Fang, *Medicinal Chemistry of Bioactive Natural Products*, John Wiley & Sons, 2006.

G. Brahmachari, *Bioactive Natural Products*: *Chemistry & Biology*, Wiley-VCH, 2015.

S. Hanessian, *Natural Products in Medicinal Chemistry: Methods and Principles in Medicinal Chemistry*, Wiley-VCH, 2014.
G. Brahmachari, *Handbook of Pharmaceutical Natural products , Vols. 1 and 2*, Wiley-VCH, 2010.
G. Brahmachari, *Chemistry and Pharmacology of Naturally Occurring Bioactive Compounds*, CRC Press, Taylor & Francis, 2013.
G. Brahmachari, *Bioactive Natural Products: Opportunities and Challenges in Medicinal Chemistry*, World Scientific Publishing Co., 2011.
X. -T. Liang and W. -S. Fang, *Medicinal Chemistry of Bioactive Natural Products*, John Wiley & Sons, 2006.
G. Thomas, *Fundamentals of Medicinal Chemistry,* 5th Edn, Oxford University Press, 2013.
R. B. Silverman, *The Organic Chemistry of Drug Design and Drug Action*, 3rd Edn, Academic Press, 2014.
M. P. S. Ishar and A Faruk, *Syntheses of Organic Medicinal Compounds*, Alpha Science, 2006.
D. R. Budman, A. H. Calvert and E. K. Rowinsky, *Handbook of Anticancer Drug Development*, Lippincott Williams & Wilkins, Philadelphia, PA, USA, 2003.
E. Garrett-Meyer, *Principles of Anticancer Drug Development*, Springer, 2010.

Semester-III

Theoretical Papers (For Each, Full Marks: 50; Credit: 4)

MSCCHEMC301: Advanced Inorganic Chemistry General

Unit I

Course Objective: To give Basic knowledge of bond and band concept from molecular orbital theory. To provide the concept of Brilloin zone, band gap, etc. Classical and quantum mechanical concept of band theory, and their application with respect to electrical and thermal transport etc. Give a complete idea of semiconductors, p-n junction and superconductors etc. To get a clear idea of stoichiometric and catalytic reactions. To get a clear understanding about molecular magnetism.

Learning Outcome: Students can gather a vast knowledge of band theory of solids, semiconductors and thermal and electrical transport mechanism. To understand the band structure of non-transition and transition metal band and their subsequent properties. Concept of Hall effect to detect the type of semiconductor.

Course Content:

1. Structure and properties of solids (13 lectures)

Fundamentals, ionic, covalent, metallic hydrogen bonded and molecular solids; perovskite, ilmenite and rutile; spinel and inverse spinel, diamond cubic, silicates: single/double chain, 3D network, pyroxene, amphibole, talc, mica, clay, zeolite; crystal defects, non-stoichiometric compounds; electronic properties of solids, F-centre, conductors, insulators, semiconductors, superconductors; ferroelectricity, antiferroelectricity, pyroelectricity, piezoelectricity, liquid crystals, cooperative magnetism.

2. Metal ion promoted reactions (12 lectures)

Fundamentals, simple cycle, catalytic cycle, pliancy of substrates, Tolman catalytic loop, homogeneous/heterogeneous catalysis: Wacker-Smidt synthesis, Monsanto acetic acid process, hydrogenation by Wilkinson's catalyst, water gas shift reaction (WGSR), Fischer-Tropsch synthesis, hydrosilation, hydrophosphilynation, hydroamination, hydrocyanation and hydroboration reactions, reactions on inorganic functional groups

Unit II

3. Molecular magnetism I (13 lectures)

Classification of magnetic materials, van Vleck equation and its application, Curie-Weiss law and its implication, Lande interval rule, microstates, multiplet, multiplet width, hole formalism, zero-field splitting, spin-orbit coupling, quenching of orbital contribution, Fermi contact and pseudo-contact shifts, chemical shift reagent

4. Supramolecular Chemistry I (12 lectures)

Concept and language, scientific/technological landscape, building block, atomic and molecular valences, supramolecular orbitals, pallet of non-covalent forces and their harnessing towards crystal engineering, structure directed supramolecular arrays, crystal synthesis, deliberate isolation of different functional materials

Suggested books

A. F. Wells, *Structural Inorganic Chemistry,* 5th Edn, Oxford University Press, Oxford, 1984.

W. A. Harrison, *Electronic Structure and the Properties of Solids: The Physics of the Chemical Bonds*, Dover Publications, New York, 1989.

D. M. Adams, *Inorganic Solids*, Wiley, New York, 1992.

T. C. W. Mak and G. -D. Zhou, *Crystallography in Modern Chemistry*, Wiley, New York, 1992.

S. R. Elliot, *The Physics and Chemistry of Solids*, John Wiley & Sons, Chichester, 1998.

M. Cox, *Optical Properties of Solids,* Oxford University Press, Oxford, 2001.

L. E. Smart and E. A. Moore, *Solid State Chemistry: An Introduction,* 4th Edn, CRC Press, Boca Raton, FL, 2012.

A. R. West, *Solid State Chemistry and Its Application*, 2nd Edn, Wiley-VCH, Weinheim, 2014.

G. W. Parshall, *Homogeneous Catalysis*, Wiley, New York, 1980.

C. N. Satterfield, *Heterogeneous Catalysis in Practice*, McGraw-Hill, New York, 1980.

O. N. Temkin, *Homogeneous Catalysis with Metal Complexes: Kinetic Aspects and Mechanisms*, John Wiley & Sons, New York, 2012.

M. Beller, A. Renken and R. A. van Santen, *Catalysis,* Wiley, New York, 2012.

M. M. Rieger and L. D. Rheis (Eds), *Surfactants in Cosmetics,* Marcel Dekker Inc, New York, 1997.

M. N. Khan, *Miceller Catalysis,* Taylor and Francis Group, New York, 2007.

O. Kahn, *Molecular Magnetism*, VCH, New York, 1993.

P. Day and A. E. Underhill (Eds), *Metal-organic and Organic Molecular Magnets*, RSC, London, 2000.

J. S. Miller and M. Drillon (Eds), *Magnetism: Molecules to Materials, V; Molecule-based Magnets*, Wiley-VCH, Weinheim, 2005.
F. E. Mabbs and D. J. Machin, *Magnetism and Transition Metal Complexes*, Dover Publications, New York, 2008.
R. Winpenny (Ed), *Single-Molecule Magnets and Related Phenomena*, Structure and Bonding Series, Vol 122, Springer, Berlin, 2010.
B. D. Cullity and C. D. Graham, *Introduction to Magnetic Materials*, 2nd Edn, John Wiley & Sons, New York, 2011.
D. Gatteschi, R Sessoli and J. Villain, *Molecular Nanomagnets*, Oxford University Press, Oxford, 2006.
R. Hilzinger and W. Rodewald, *Magnetic Materials*, Wiley, New York, 2013
F. Vogtle, *Supramolecular Chemistry: An Introduction*, Wiley, Chichester, 1991.
V. Balzani and F. Scandola, *Supramolecular Photochemistry*, Ellis Horwood, Chichester, 1991.
J. -M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, VCH, Weinheim, 1995.
G. A. Jeffrey, *An Introduction to Hydrogen Bonding,* Oxford University Press, Oxford, 1997.
S. T. Hyde, B. Ninham, S. Anderson, Z. Blum, T. Landh, K. Larsson and S. Liddin, *The Language of Shape*, Elsevier, Amsterdam, 1997.
C. N. R. Rao, A. Muller and A. K. Cheetham, *Nanomaterials Chemistry: Recent Developments and New Directions*, Wiley-VCH, Weinheim, Germany, 2007.
C. C. Koch, *Nanostructured Materials Processing, Properties, and Applications*, William Andrew Inc, 2007.
J. W. Steed and J. L. Atwood,*Supramolecular Chemistry*, 2nd Edn, John Wiley & Sons, New York, 2009.
K. Rurack and R. Martinez-Manez (Eds), *The Supramolecular Chemistry of Organic-Inorganic Hybrid Materials,* John Wiley & Sons, Hoboken, New Jersey, 2010.
E. R. T. Tiekink and J. Zukerman-Schpector (Eds), *The Importance of Pi-Interactions in Crystal Engineering: Frontiers in Crystal Engineering*, 1st Edn, John Wiley & Sons, Chichester, 2012.

MSCCHEMC302: Advanced Organic Chemistry General

Course Objectives: Green chemistry is an area of chemistry and chemical engineering focused on the designing of products and processes that minimize the use and generation of hazardous substances. There are various scope of green chemistry. To learn various organic reactions and reagents used in them as tools applied in the art of organic synthesis. To learn retrosynthetic approach towards organic synthesis. To learn about various types of pericyclic reactions including cycloaddition, electrocyclic reactions and sigmatropic rearrangement.

Teaches the chemistry involved in various photochemical reactions & their basic principles which enables students to learn a variety of photochemical reactions, their mechanisms; to understand and explain photochemical and photophysical processes and their quantum yield expressions, understanding the selection rules for electronic transitions and develop quantum mechanical formulation of Franck-Condon principle, to understand and explain the properties of electronically excited molecules, to understand and explain the nonradiative intramolecular electronic transitions, very scoring chapter from competitive point of view.

Learning Outcomes: It affects our environment and at the same time it is very beneficial to our society. Human health, environment, economy and business are benefitted through the study of green chemistry.

At the end of the course, the learners should be able to: Use various reagents and organic reactions in a logical manner in organic synthesis; use retrosynthetic method for the logical dissection of complex organic molecules and devise synthetic methods.

After completing the chapter pericyclic reactions, the learners should be able distinguish mechanistic difference between a perycyclic and an ionic reactions. They should be able to design synthetic scheme of various commercial or non-commercial chemicals by using the concept of pericyclic reactions.

After completing the chapter photochemistry, the student will be expected to be able to: Explain fundamentals of photochemistry and the laws governing it; Explain Jablonski diagram and describe and radiative and non-radiative transitions; Describe photophysical kinetics of unimolecular and bimolecular processes. Determine life time, redox potential, dipole moment, pK values, etc. of electronically excited molecules.

Unit I

1. Green chemistry: Concept, practice and aspects in current synthetic chemistry (08 lectures)

The concept and ‘Twelve Principles’ of green chemistry; current-day need in chemical and industrial sectors; atom-economy; choice of catalysts, solvents, energy consideration and reaction media, and eco-friendliness and sustainability of a chemical process; tools of green chemistry; real-world cases of practicing green chemistry

2. Organic synthesis focusing on carbon-heteroatom bonds (17 lectures)

Organoboron chemistry: Chemistry of organoboron compounds, carboranes, hydroboration, reactions of organoboranes, unsaturated hydrocarbon synthesis, allyl boranes, boron enolates; *Organosilicon chemistry*: Chemistry of organosilicon compounds, synthetic uses of silyl ethers, silylenol ethers, TMSCN, alkene synthesis, alkynyl, vinyl, aryl, allyl and acyl silanes; Brook rearrangement, silicon Baeyer-Villiger rearrangement; *Organophosphorous chemistry*: Chemistry of organophosphorus compounds, phosphorus ylides – Wittig reaction and itsmodifications, phosphine oxides and its applications; *Organosulphur chemistry*: Chemistry of organosulphur compounds, sulphur- stabilized anions and cations, sulphonium salts, sulphonium and sulphoxonium ylides

Unit II

3. Protection-deprotection and retrosynthetic strategy applied in organic reactions (10 lectures)

Protection-deprotection: Principle of protection-deprotection and its role in organic synthesis, differentmethods for protection-deprotection of common functional groups (alcoholic and phenolic hydroxyl(s), amino, carbonyl and carboxylic groups)

Retrosynthetic strategy: The disconnection approach – basic principles, one-group and two-group disconnections; strategies of retrosynthesis; retrosynthetic analysis for ibogamine, valeranone, squalene, estrone, progesterone and ginkgolide B

4. Pericyclic reaction I (09 lectures)

Definition and classification of pericyclic reactions; methods of analyzing pericyclic reactions (Molecular Orbital Symmetry Correlation Method, Frontier Orbital Method (FMO), and Transition State Aromaticity Method); *Electrocyclic reactions*: Definition, classification, Woodward-Hoffmann Rules for electrocyclic reactions, examples of different types of electrocyclic reactions (three-, four-, five- six-, seven- and eight-membered ring systems); *Cycloaddition reactions*: Definition, classification, Woodward-Hoffmann Rules for cycloaddition reactions, examples of different types of cycloaddition reactions – [2π + $2\ \pi$]-cycloadditions, [4π + $2\ \pi$]-cycloadditions, dienes and dienophiles, Diels-Alder reaction, '*cis*' rule, Alder's '*endo*' rule, regioselectivity, 1,3-dipolar cycloadditions, higher order cycloadditions ([4π + $4\ \pi$]-, [6π + $4\ \pi$]-, [8π + $2\ \pi$]- and [14π + $2\ \pi$]-cycloadditions).

5. Organic photochemistry I (06 lectures)

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, *Cis-trans* isomeriation, Paterno-Buchi reaction, Norrish type I and II reactions, di-pi-methane rearrangement, photochemical reactions of carbonyl compounds

Suggested books

P. T. Anastas and J. C. Warner, *Green Chemistry: Theory and Practice*, Oxford University Press, 2000.

P. T. Anastas (Series editor), *Handbook of Green Chemistry*, Wiley-VCH Book Series

James H Clark (Series Editor-in-Chief), *RSC Green Chemistry*, Royal Society of Chemistry Book Series

V. K. Ahluwalia and K. Kidwai, *New Trends in Green Chemistry*, Springer, 2004.

R. A.Sheldon, Arends, I.and U. Hanefeld, *Green Chemistry and Catalysis*, Wiley-VCH, 2007.

M. Doble and A. K. Kruthiventi,*Green Chemistry and Engineering*, Academic Press, 2007.

G. Brahmachari, *Green Synthetic Approaches for Biologically Relevant Heterocycles*, Elsevier, 2014.

V. K. Ahluwalia, *Green Chemistry: Environmentally Benign Reaction*, Ane Books, 2006.

V. M. Kolb, *Green Organic Chemistry and its Interdisciplinary Applications*, CRC Press, 2016.

S. K. Sharma and A. Mudhoo, *Green Chemistry for Environmental Sustainability*, CRC Press, 2010.

A. P. Dicks, *Green Organic Chemistry in Lecture and Laboratory*, CRC Press, 2011.

S. A. Henrie, *Green Chemistry Laboratory Manual for General Chemistry*, CRC Press, 2015.

J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, 2001.

F. A. Carry and R. J. Sundberg, *Advanced Organic Chemistry – Part-A and B*, 5th Edn, Springer, 2007.

L. G. Wade, Jr. and M. S. Singh, *Organic Chemistry*, 6th Edn, Pearson Education, 2008.

T. G. Graham and C. B. Fryhle, *Organic Chemistry*, 8th Edn, John Wiley & Sons, 2004.

R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, *Organic Chemistry*, 7th Edn, Pearson Education, 2013.

M. Schlosser and K. Smith, *Organoboron Chemistry*, Wiley-VCH, 2013.

M. G Davidson, K. Wade, T B Marder and A.K Hughes (Editors), *Contemporary Boron Chemistry*, Royal Society of Chemistry, 2000.

B. Marciniec, *Progress in Organosilicon Chemistry*, Taylor & Francis, 1995.

N. Auner and J. Weis (editors), *Organosilicon Chemsitry III: From Molecules to Materials*, Wiley-VCH, 1998.

G. H. Whitham, *Organosulfur Chemistry*, Oxford University Press, 1995.

R. J. Cremlyn, An Introduction to Organosulfur Chemistry, Wiley-VCH, 1996.

R. Engel, Handbook of Organophosphorous Chemistry, CRC Press, 1992.

L. D. Quin, *A Guide to Organophosphorus Chemistry*, Wiley-VCH, 2000.

D. W Allen, D. Loakes and J. C Tebby (Series Editors), *Organophosphorous Chemistry*, RSC Book Series.

P. G. M. Wuts and T. W. Greene, *Greene's Protective Groups in Organic Synthesis*, 4th Edn, Wiley-VCH, 2006.

S. Warren and P. Wyatt, *Organic Synthesis: The Disconnection Approach*,2nd Edn, Wiley-VCH, 2008.

E. J. Corey and X.-M. Chelg, *The Logic of Organic Synthesis*, John Wiley & Sons, 1995.

T.L. Gilchrist and R.C. Storr,*Organic Reactions and Orbital Symmetry*, 2ndEdn., Cambridge University Press, 1979.

N. J. Turro,*Modern Molecular Photochemistry*, The Benjamin/ Cummings Publishing Co., Inc., 1978.

R. B. Woodward and R. Hoffman, *The Conservation of Orbital Symmetry*, Academic Press, 1970.

J.M. Coxon and B.H. Halton, *Organic Photochemistry*, Cambridge University Press, 1974.

S. Sankararaman,*Pericyclic Reactions – A Textbook*, Wiley-VCH Verlag, 2005.

MSCCHEMC303: Advanced Physical Chemistry General

Unit I

1. Applications of group theory in chemistry (13 lectures)

Molecular vibrations, Normal mode analysis, symmetry of normal modes, Selection rules for infrared and Raman spectra, Hybridization, Construction of Symmetry adapted linear combination of atomic orbitals (SALC), Molecular orbital description of different organic, inorganic and organometallic molecules.. Application of group theory to ligand and crystal field theory, construction of energy level diagrams, correlation diagrams. Symmetry and chemical reactions; Woodward-Hoffmann rules.

Objective: In this segment, we have discussed how Group Theory is used to construct molecular orbitals and energy levels of several π-conjugated molecules & type molecules. Allowedness/forbiddenness of several spectroscopic transitions, prediction of hybridization, Bond order have been demonstrated in terms of Group Theory. In this chapter a discussion on the classification of normal modes of molecular vibrations & their infrared and Raman activities have been done considering the basic principles of Group Theory. n AB

Learning Outcome: In NET/SET/GATE examinations, there are several questions from the application part of the Group Theory.

2. Crystallography and surface chemistry (12 lectures)

Crystal symmetry, translation, glide plane and screw axis, Bravis lattice, space groups and its determination, stereographic projection, Fourier series, electron density and structure factor, methods for solving the phase problems, Bzones and Fermi level in lattice, concept of particle-hole in conduction process, band theory, theory of conductors, semiconductors and insulators.

Solid surfaces: External and internal surfaces; Bulk and surface structure of FCC, BCC and HCP metals; Notation of surface structures; Relaxation and reconstruction of surfaces; homogeneous and heterogeneous surfaces. Solid-gas interfaces: Types of adsorption; Adsorption isotherms – Langmuir, Tempkin and BET. Determination of surface area of adsorbents; temperature dependence of adsorption isotherms.

Objective: To give Basic knowledge of bond and band concept from molecular orbital theory. To provide the concept of Brilloin zone, band gap, etc. Classical and quantum mechanical concept of band theory, and their application with respect to electrical and thermal transport etc. Give a complete idea of semiconductors, p-n junction and superconductors etc.

Course outcome: Students can gather a vast knowledge of band theory of solids, semiconductors and thermal and electrical transport mechanism. To understand the band structure of non-transition and transition metal band and their subsequent properties. Concept of Hall effect to detect the type of semiconductor.

Unit II

3. Chemistry of Polymers

(08 lectures)

Basic Concepts, classification, nomenclature, molecular weights, molecular weight distribution Methods for determination of Molecular weights, viscosity molecular weight, intrinsic viscosity, mark-Houwink relationships, Glass transition temperature, Polymerization reaction, kinetics of free radical and condensation polymer. Graft polymerization. Morphology and crystallinity of polymer by TGA and SEM analysis.Criteria for polymer solubility.Thermodynamics of polymer solutions.Theta temperature.Flory-Huggins model, dilute polymer solution.Excluded volume.

Course objectives

* To understand theory of polymerization and determination of molecular weight of polymer.

* To understand kinetics of polymerization.

* To understand theories of polymer solutions.

Learning outcomes

After completing the course the student will be expected to be able to:

• determine molecular weight of polymer.

• determine rate / degree / extent of polymerization.

• explain behavior of polymer in solution.

4. Biophysical chemistry (08 lectures)

Structure and functions of proteins and nucleic acids, Hydrophobic effect and micelle formation, hydrophobic interaction, stabilization and denaturation of protein. Water structure alternation theory of denaturation of protein, protein–lipid interaction, Transport of ions and small molecules through membranes. Ion channels.

Course objectives

* To understand the structure of micelles, proteins and nuclic acids

* To understand protein denaturation mechanism.

* To understand the protein-lipid interaction and transport of ions through the membranes.

Learning outcomes

After completing the course the student will be expected to be able to:

• know the structure of micelles, reverse micelles, proteins, DNA and RNA.

• know how the protein denaturates.

• know how various ions are transported into body through the membranes

5. Spectroscopy (09 lectures)

Maxwell's field equations, transition between states, selection rules and forbidden transitions; NMR: Relaxation and exchange phenomena, theories of chemical shift and nuclear spin-spin coupling in 2-spin systems with applications, pulsed NMR (spin echo); Electronic: n-π*, π- π* and CT transitions; vibrational: simple polyatomic molecules, normal modes, influence of nuclear spin on vibration-rotation spectra of polyatomics, time-resolved IR, 2-d IR, principles of 1D and 2D NMR. Principles of ESR and Mossbauer spectroscopy.

Course objectives

* To understand the basic aspects of different types of transitions

* To understand the basic aspects and application of few advanced spectroscopic techniques.

Learning outcomes

After completing the course the student will be expected to be able to:

• know about the different kinds of electronic transitions like n-π*, π- π* and CT transitions

• know about the basic principles and application of modern spectroscopic techniques like time-resolved IR, 2-d IR, principles of 1D and 2D NMR.

Suggested books

S. C. Rakshit, *Molecular Symmetry Group and Chemistry*, The New Book Stall, Kolkata, 1988.

V. Heine, *Group Theory in Quantum Mechanics: An Introduction to Its Present Usage*, Dover Publication, New York, 1991.

D. M. Bishop, *Group Theory and Chemistry*, Oxford University Press, Oxford, 1993.

A. Vincent, *Molecular Symmetry and Group Theory*, John Wiley & Sons, New York, 1998.

F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn, John Wiley & Sons, New York, 1999.

R. L. Cramer, *Molecular Symmetry and Group Theory*, Wiley, 2013.

C. Kittel, *Introduction to Solid State Physics*, 4th Edn, John Wiley & Sons, New York.

P. A. Cox, *The Electronic Structure & Chemistry of Solids*, Oxford University Press, Oxford, 1987.

M. F. C. Ladd and R. A. Palmer, *Structure Determination by X-ray Crystallography*, 3rd Edn, Plenum Press, New York, 1994.

X. Clegg, *Crystal Structure Determination*, Oxford University Press, Oxford,

A. R. West, Basic Solid State Chemistry, Wiley

G. A. Somorjai, Y Li., Introduction to Surface Chemistry and Catalysis, Wiley.

W. Adamson, *Physical Chemistry of Surfaces*, John Wiley & Sons, New York, 1990.

H. -J. Butt, K. Graf and M. Kappl, *Physics and Chemistry of Interfaces*, Wiley-VCH, 2003.

J. H. Clint, *Surface Chemistry*, Blackie and Son Ltd, 1992.

P. W. Atkins, *Physical Chemistry*, Oxford University Press, Oxford, 1998.

R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, Oxford University Press, Oxford, 2000.

P. J. Flory, Principles of Polymer Chemistry, Cornell University Press.

C. Tanford, *Physical Chemistry of Macromolecules*, John Wiley & Sons, Inc, New York, 1961.

F. W. Billmeyer, *Text Book of Polymer Science*, 2nd Edn, Wiley-Interscience, New York, 1971.

G. S. Mishra, *Introductory Polymer Chemistry*, Wiley Eastern, New Delhi, 1993.

S. F. Sun, *Physical Chemistry of Macromolecules: Basic Principles and Issues*, John Wiley & Sons, New York, 1994.

J. P. Allen, Biophysical Chemistry, Wiley

I. N. Levine, Quantum Chemistry: Molecular Spectroscopy,

G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill International Book Company, Tokyo, 1982.

W. Kemp, *NMR in Chemistry: A Multinuclear Approach*, Macmillan Press, Hong Kong, 1986.

R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.

J. K. M. Sanders, E. C. Constable and B. K. Hunter, *Modern NMR Spectroscopy: A Workbook of Chemical Problems*, Oxford University Press, Oxford, 1993.

C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1994.

H. Gunther, *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, Wiley, New York, 1995.

A. Abragam and B. Bleaney, *Electron Paramagnetic Resonance of Transition Metal Ions*, Clarendon Press, Oxford, 1970. N. M. Atherton, *Principles of Electron Spin Resonance*, Ellis Horwood/Prentice-Hall, Hemel Hempsted, 1993.

Major Electives (any one)

MSCCHEMMJE301: Inorganic Chemistry Major I

Course Objective: Synthetic methodology will play crucial role in the synthesis of ligand complexes as well as materials. Various constrained of the process will also be understood. The learners should be able to apply theories of chemical bonding, reaction mechanism, electronic structure and magnetic properties of coordination complexes to identify the occurrence, active site structure and functions of some transition metal ions.

Learning Outcome: Such course will be very useful for the synthesis and design for ligand and complexes and at the same time various research field will be explored. At the end of the course, the learners should be able to: Identify the principles, structure and reactivity of selected coordination complexes and interpret their electronic spectra and magnetic properties.

Unit I

1. Synthetic methodology in inorganic, coordination and organometallic chemistry (15 lectures)

Ligand design/synthesis, ligand topology, molecular mechanics/engineering, tailoring/appending of pendant arm; coordination compound design/synthesis using classical/benign method, self-assembly, atom economy, thermolysis, photolysis, sonolysis, electrolysis, sol-gel method, hydrothermal method, cryochemistry, top-down and bottom-up methods for nano-structured solids.

2. Organometallic chemistry II (10 lectures)

Reactions occurring in metal-bound state: ligand substitution, oxidative addition, reductive elimination; reactions triggered by modification on ligand framework: insertion and deinsertion, ligand-based nucleophilic addition, nucleophilic abstraction, electrophilic reactions; applications to organic synthesis: enantioselective functional group interconversion, chiral synthesis, protection and deprotection; transmetallation and cyclisation reactions, bioorganometallics, organo-dendrimer, surface organometallic chemistry

Unit II

3. Spectral (IR, NMR, EPR, UV-Vis Mossbauer, etc.) studies of inorganic, coordination and organometallic species (25 lectures)

Fundamentals, elucidation of geometric structure, electronic structure, stereochemistry, bonding, molecular aggregate, superstructure and reaction pathway in halide, pseudohalide, carbonyl, nitrosyl, DMSO, polypyridine, azoheterocycle, oxime, quinone, macrocycle containing compounds and organometallic complexes; enumeration and characterization: geometrical (*cis*/*trans*, *fac*/*mer*) and stereo (optical) isomers in different polyhedra; ligational motif and chelate loop, structural distortion, effective pi-acceptance centre, oxidation state, spin state, redox site of non-innocent ligands, mu-bonding and hapticity, electrophilicity/nucleophilicity, quasi- and superaromaticity, fluxionality, matalloligand, probing chemical reactivity and reaction pathways (intramolecular/intermolecular, stereoretentivity/stereodynamicity), covalency of ML bonding and comment on bonding theories

Suggested books

L. S. Hegedus, *Transition Metal in the Synthesis of Complex Organic Molecules*, University Science Press, Mill Valley, CA, 1994.

G. Wulfsberg, *Inorganic Chemistry*, Viva Books Private Ltd, New Delhi, 2001.

W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, 4th Edn, Cambridge University Press, Cambridge, 2004.

G. Rothenberg, *Catalysis: Concepts and Green Applications*, Wiley-VCH, Weinheim, 2008.

H. -D. Höltje, W. Sippl, D. Rognan and G. Folkers, *Molecular Modeling: Basic Principles and Applications*, 3rd Edn, Wiley-VCH, Weinheim, 2008.

J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, 2nd Edn, John Wiley & Sons, New York, 2009.

R. Xu, W. Pang and Q. Huo (Eds), *Modern Inorganic Synthetic Chemistry*, Elsevier, New York, 2011.

A. Yamamoto, *Organotransition Metal Chemistry*, Wiley, New York, 1986.

J. P. Collmann, L. S. Hegedus, J. R. Norton and R. G. Finke, *Principles and Applications of Organotransition metal Chemistry*, University Science Books, Mill Valley, CA, 1987.

R. G. Wilkinns, *Kinetics and Mechanism of Reactions of Transition Metal Complexes*, 2nd Edn, VCH, Weinheim, 1991.

R. H. Crabtree, *The Organomettalic Chemistry of the Transition Metals*, 2nd Edn, Wiley, New York , 1994.

L. S. Hegedus, *Transition Metal in the Synthesis of Complex Organic Molecules*, University Science Press, Mill Valley, CA, 1994.

G. O. Spessard and G. L. Miessler, *Organometallic Chemistry*, Prentice-Hall, New Jersey, 1997.

R. B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems*, Oxford University Press, Oxford, 1998.

R. V. Eldik and C. D. Hubbard (Eds) *Advances in Inorganic Chemistry*, Vol 54, Academic Press, New York, 2003.

R. H. Crabtree, *The Organomettalic Chemistry of the Transition Metals*, 4th Edn, Wiley, New York, 2005.

D. Steinborn, *Fundamentals of Organometallic Catalysis*, John Wiley & Sons, New York, 2011.

G. Aruldhas, *Molecular Structure and Spectroscopy*, 2nd Edn, Prentice-Hall of India, New Delhi, 2007.

D. N. Sathyanarayana, *Electronic Absorption Spectroscopy and Related Techniques*, University Press, 2001.

D. Shillady, *Essentials of Physical Chemistry*, CRC Press, Boca Raton, FL, 2012.

A. B. P Lever, *Inorganic Electronic Spectroscopy*, Elsevier, New York, 1984.

Raton, FL, 2008.

H. H. Jaffe and M. Orchin, *Symmetry, Orbitals and Spectra*, Wiley, New York, 1982.

K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, Part B, 6th Edn, John Wiley & Sons, New Jersey, 2009.

B. Schrader (Ed) Infrared and Raman Spectroscopy: Methods and Applications, VCH Weinheim, 1995.

W. Henderson and J. S. McIndoe, *Mass Spectrometry of Inorganic, Coordination and Organometallic Compounds: Tools-Techniques-Tips*, John Wiely & Sons, Ltd, Chichester, 2005.

H. Gunther, *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, Wiley, New York, 1995.

N. M. Atherton, *Principles of Electron Spin Resonance*, Ellis Horwood/Prentice-Hall, Hemel Hempsted, 1993.

E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, *Structural Methods in Inorganic Chemistry*, 2nd Edn, Blackwell Scientific Publications, Oxford, 1991.

J. E. Wertz and J. R. Boulton, *Electron Spin Resonance: Elementary Theory and Practical Applications*, Chapman and Hall, London, 1986.

J. Garcia Sole, L. E. Bausa and D. Jaque, *An Introduction to the Optical Spectroscopy in Inorganic Solids*, John Wiley & Sons, New York, 2005.

MSCCHEMMJE302: Organic Chemistry Major I

Course Objectives: Green chemistry is an area of chemistry and chemical engineering focused on the designing of products and processes that minimize the use and generation of hazardous substances. There are various scope of green chemistry.

To learn various organic reactions and reagents used in them as tools applied in the art of organic synthesis. To learn retrosynthetic approach towards organic synthesis.

To learn about various types of pericyclic reactions including cycloaddition, electrocyclic reactions and sigmatropic rearrangement.

Teaches the chemistry involved in various photochemical reactions & their basic principles which enables students to learn a variety of photochemical reactions, their mechanisms; to understand and explain photochemical and photophysical processes and their quantum yield expressions, understanding the selection rules for electronic transitions and develop quantum mechanical formulation of Franck-Condon principle, to understand and explain the properties of electronically excited molecules, to understand and explain the nonradiative intramolecular electronic transitions, very scoring chapter from competitive point of view.

Learning Outcomes: It affects our environment and at the same time it is very beneficial to our society. Human health, environment, economy and business are benefitted through the study of green chemistry. At the end of the course, the learners should be able to: Use various reagents and organic reactions in a logical manner in organic synthesis and use retrosynthetic method for the logical dissection of complex organic molecules and devise synthetic methods.

After completing the chapter pericyclic reactions, the learners should be able distinguish mechanistic difference between a perycyclic and an ionic reactions. They should be able to design synthetic scheme of various commercial or non-commercial chemicals by using the concept of pericyclic reactions.

After completing the chapter photochemistry, the student will be expected to be able to: Explain fundamentals of photochemistry and the laws governing it. Explain Jablonski diagram and describe and radiative and non-radiative transitions. Describe photophysical kinetics of unimolecular and bimolecular processes. Determine life time, redox potential, dipole moment, pK values, etc. of electronically excited molecules.

Unit I

1. VBT and MOT: Concept, molecular structure and reactivity (05 lectures)

Orbitals, atomic orbitals, hybridization of atomic orbitals, HOMO, LUMO, molecular structure and reactivity – Basic concepts and understanding with the help of Valence Bond Theory (VBT) and Molecular Orbital Theory (MOT)

2. Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD) (05 lectures)

Chiroptical properties of organic molecules; ORD and CD principles and applications; ORD and CD curves: Cotton effect; empirical and semiemperical rules

3. Asymmetric synthesis (15 lectures)

Principles and newer methods of asymmetric synthesis (including enzymatic and catalytic nexus); enantio- and diastereoselective synthesis;reactions of enolates (α−substitution);addition to C=C double bonds (electrophile- induced cyclisation, iodolactonisation, hydroboration, conjugate additions); asymmetric hydrogenation with special reference to Ru-BINAP catalysts; asymmetric reduction of prochiral ketones with Baker's Yeast and CBS-catalyst; asymmetric epoxidation with special reference to Sharpless and Jacobsen epoxidation; asymmetric aldol reactions, asymmetric Michael reaction; Few important industrial applications of asymmetric synthesis

Unit II

4. Chemistry of heterocyclic compounds: Synthesis, properties and reactions (15 lectures)

Nomenclature of bicyclic and tricyclic fused systems;heterocyclic synthesis – principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions; synthesis and reactivity of 3-, 4-, 5- 6- & 7-membered heterocycles with one, two or more heteroatoms (aziridines, oxiranes, thiiranes, azetidines, oxetanes, thietanes, diazines, triazines, thiazines, azepines, oxepines); benzo-fused five and six-membered heterocycles - synthesis and reactions including medicinal applications of benzopyrroles, benzofurans, benzothiophenes, quinolizinium and benzopyrylium salts, coumarins and chromones; phosphorus and selenium containing heterocycles;role of heterocyclic compounds in biological systems; heterocycles in pharmaceutical industry.

5. Organometallic chemistry (10 lectures)

Application of transition metals in organic synthesis – preparative, structural and mechanistic aspects; Davies rule, catalytic nucleophilic addition and substitution reactions;coupling reaction – Heck, Stille, Suzuki coupling Ziegler Naata reaction;olefin metathesis; Tebbe's reagent, Pauson-Khand reactions; Volhsrdt co-trimerisation, functional organometallic compounds; use of non-transition metals- Indium, tin, zinc in organic synthesis

Suggested books

E. V. Anslyn and D. A. Dougherty,*Modern Physical Organic Chemistry*, University Science Books, 2006.

S. Shaik, and P. C. Hiberty, (2004) *Valence Bond Theory, Its History, Fundamentals, and Applications: A Primer, In: Reviews in Computational Chemistry*, Volume 20 (eds. K. B. Lipkowitz, R. Larter and T. R. Cundari), John Wiley & Sons, Inc., Hoboken, NJ, USA, 2004.

F. A. Carroll, *Perspectives on Structure and Mechanism in Organic Chemistry,* 2nd Edn, Wiley-VCH, 2011.

P. Crabbe, *ORD and CD in Chemistry and Biochemistry*, Academic Press, 1972.

E. L. Eliel, S. H. Wilson and L. N. Mander,*Stereochemistry of Organic Compounds*, John Wiley & Sons, Inc., 2003.

D. Nasipuri, *Stereochemistry of Organic Compounds (Principles and Applications),* 2nd Edn, Wiley Eastern Limited, New Delhi, 1994.

R. E. Gawley and J. Aube, *Principles of Asymmetric Synthesis*, Elsevier, 1996.

M. Gruttadauria and F. Giacalone, Catalytic Methods in Asymmetric Synthesis: Advanced Materials, Techniques, and Applications, John Wiley & Sons, 2011.

I. Ojima, *Catalytic Asymmetric Synthesis*, John Wiley & Sons, 2013.

G.-Q. Lin, Y.-M.Li and A. C. Chan, Principles and Applications of Asymmetric Synthesis, John Wiley & Sons, 2003.

A. M. P. Koskinen, *Asymmetric Synthesis of Natural Products*, John Wiley & Sons, 2012.

J. A. Joule and K. Mills, Heterocyclic Chemistry, Blackwell Science Publication, 2000.

R. K. Bansal,*Heterocyclic Chemistry: Syntheses, Reactions and Mechanisms*, Wiley Eastern Limited, New Delhi, 1999.

T. L. Gilchrist, *Heterocyclic Chemistry*, Pearson Education, 2008.

T. Eicher, S. Hauptmann and A. Speicher, *TheChemistry of Heterocycles*, Wiley-VCH, 2012.

G. Brahmachari, *Green Synthetic Approaches for Biologically Relevant Heterocycles*, Elsevier, 2014.

A. I. Meyers, Heterocycles in Synthesis, John Wiley & Sons, 1974.

A.R. Katritzky, *Comprehensive Heterocyclic Chemistry*, Elsevier Book series.

R. C. Mehrotra, *Organometallic Chemistry*, New Age International., 2007.

G. O. Spessard and G. L. Miessler, *Organometallic Chemistry*, oxford University Press, 2010.

B. D. Gupta, *Basic Organometallic Chemistry: Concepts, Syntheses and Applications*, Universities Press, 2011.

D. Astruc, *Organometallic Chemistry and Catalysis*, Springer, 2007.

MSCCHEMMJE303: Physical Chemistry Major I

Course objectives

- To understand the concept of ensembles. Types of ensembles
- To understand Maxwell-Boltzmann (MB), Bose-Einstein (BE) and Fermi-Dirac (FD) distributions and derivation of thermodynamic relations.

Learning outcomes After completing the course the student will be expected to be able to:

- explain microcanonical, canonical and grand canonical ensembles.
- derive Maxwell-Boltzmann (MB), Bose-Einstein (BE) and Fermi-Dirac (FD) distribution laws.
- explain and calculate the values of thermodynamic properties.
- explain black body radiation and photon gas.

Unit I

1. Classical mechanics (10 lectures)

Newtons' prescription for classical mechanics, Laws of motion: law of inertia, law of causality, Superposition principle of force, introduction to the idea of law of force for motion, Conservative and non-conservative force, definition of potential energy, conservation of total mechanical energy for conservative system and its implication, principle of least action, generalized coordinate systems, Legendre transformation, Poission bracket Lagrangian equation of motion and definition of generalized momentum, Hamiltonian equation of motion.

2. Approximate methods in quantum chemistry (15 lectures)

Variation theorem, application to ground states of various systems. Linear variation method, Secular determinant, Introduction to matrix mechanics-eigen values and eigen vectors, Variation method for excited states. Time-independent perturbation theory for nondegenerate states, Perturbation of a two-level system, Many level systems, Degenerate perturbation theory and Stark effect, Hellman-Feynman and Virial Theorems. Time-dependent perturbation theory, Rabi Oscillation, Many level system; the variation of constants, the effect of slowly switched constant perturbation, The effect of oscillating perturbation, Transition rates to continuum, A semi-classical treatment to radiation-matter interaction. Fermi Golden rule, Einstein transition probabilities, lifetime and energy uncertainty.

Unit II

3. Statistical Mechanics (25 Lectures)

Concept of Ensemble. A priori probability. Gibbs postulate in Statistical mechanics. Ergodic hypothesis. Prescription for studying of thermodynamic systems based on ensemble method. Preparation of equilibrium ensemble corresponding to given thermodynamic system (isolated, closed and open).Determination of distribution function.Partition function.Calculation of thermodynamic properties in terms of partition function.Theory of Fluctuations. Calculation of fluctuation in energy, number of particles, density, entropy, volume, temperature etc The classical partition function. Phase space and the Liouville equation

Boltzmann, Fermi-Dirac and Bose-Einstein Statistics Canonical partition function for non-interacting distinguishable and non-identical particles. Boltzmann Statistics. Grand canonical partition function for non-interacting identical particles. Fermi-Dirac and Bose-Einstein statistics and their limiting behavior.Ideal monoatomic gas.The translational partition function.The electric and nuclear partition function.Thermodynamic function.Ideal diatomic gases.The rigid rotor-Harmonic oscillator approximation.The vibrational partition function. The rotational partition function of a heteronuclear molecule. The symmetry requirement of the total wave function of a homonuclear diatomic molecule. The rotational partition function of a homonuclear diatomic molecule. Thermodynamic functions. A weakly degenerate ideal Fermi-Dirac Gas. A strongly degenerate ideal Fermi-Dirac gas. A weakly degenerate ideal Bose-Einstein gas.A strongly degenerate ideal Bose-Einstein gas. An ideal gas of photons.Einstein and Debye theory of Specific heat capacity of solids.Equilibrium Constants in terms of partition functions.Imperfect gases, The Virial equation of state from the grand partition functions.The expression for second Virial co-efficient.

Suggested books

R. P. Feynman, R. P. Leighton and M. Sands, The Feynman Lectures on Physics, Narosa, New Delhi.

N. C. Rana, P. S. Joag, Classical Mechanics, Mcgraw-Hill Education India Pvt. Ltd., New Delhi.

H. Eyring, J. Walter and G. F. Kimball, *Quantum Chemistry*, Wiley, New York, 1944.

P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.

L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, New York, 1985.

A. K. Chandra, *Introductory Quantum Chemistry,* Tata McGraw-Hill Publishing Co, New Delhi, 1989.

F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, New Delhi, 1990.

D. A. McQuarrie, *Quantum Chemistry,* Viva Books Pvt Ltd, New Delhi, 2003.

I. N. Levine, Quantum Chemistry, PHI Learning Pvt. Ltd, New Delhi, 2010.

E. Merzbacher, Quantum Mechanics, Wiley, 1998.

F. Reif, *Fundamentals of Statistical and Thermal Physics*, McGraw-Hill, New York, 1965.

E. S. R. Gopal, *Statistical Mechanics and Properties of Matter*, Ellis Horwood, England, 1974.

S. K. Ma, *Statistical Mechanics*, World Sci, Singapore, 1985.

R. K. Pathria, *Statistical Mechanics*, Butterworth-Heinemann, 1996.

D. A. McQuarrie, Statistical Mechanics, Viva Books Pvt. Ltd.

Practical Papers (For Each, Full Marks: 50; Credit: 4)

MSCCHEMC304: Advanced Chemistry General (compulsory for all)

Course objectives

- To understand the concepts and methods of chemical analysis
- To gather hand on experience of UV-Vis, FTIR, Fluorimeter, Thermal Analyser, CHN(S) Analyser, Electrochemical Analyser, etc

Learning outcomes After completing the course the student will be expected to be able to:

- Do the instrumental chemical analysis
- Run the machines like of UV-Vis, FTIR, Fluorimeter, Thermal Analyser, CHN(S) Analyser, Electrochemical Analyser, etc

Course Content:

1. Instrumental methods in chemical analysis:use of different instruments like UV-Vis, FTIR, Fluorimeter, Thermal Analyser, CHN(S) Analyser, Electrochemical Analyser, etc in various chemical analyses and computer simulation

MSCCHEMMJE304: Inorganic Chemistry Major: Practical I

Course objectives

- To know the synthetic methods and characterizations of Schiff bases

Learning outcomes After completing the course the student will be expected to be able to:

- Synthesize the Schiff bases
- Characterization of Schiff Bases by machines like of UV-Vis, FTIR, Fluorimeter, Thermal Analyser, CHN(S) Analyser, Electrochemical Analyser, pH meter etc.

Course Content:

1. Synthesis of di-, tri- and polydentate Schiff bases and related chelators/congregators
2. Isolation of the complexes with synthesized ligands in (1) and ones commercially available
3. Spectroscopic (IR, UV-Vis, Fluorescence, etc) characterization of the ligands and complexes
4.Determination of composition and formation constants of selected systems by pH-metric and spectrophotometric methods

MSCCHEMMJE305: Organic Chemistry Major: Practical I

Course objectives

• To know the different quantitative analysis methods of organic compounds

• To know the different qualitative synthesis methods of organic compounds

Learning outcomes After completing the course the student will be expected to be able to:

• Quantitative analysis and qualitative synthesis of different organic compounds

Course Content:

1. Quantitative estimation of organic compounds

   a) Sugars (glucose, cane sugar), (b) phenol, (c) aniline, (d) acetone, (e) nitrogen by Kjldahl method, (e) saponification and iodine value of oil

2. Organic preparation (single and/or two-step process)

   Preparation of organic compoundsby conventional and green chemical methods (involving single and/or two-step process) followed by purification and characterization by spectroscopic technique

MSCCHEMMJE306: Physical Chemistry Major: Practical I

Course objectives

• To know the methods determination of dissociation constants by conductivity measurement and potentiometric titration

Learning outcomes After completing the course the student will be expected to be able to:

• Determine dissociation constants by conductivity measurements and potentiometric titrations

Course Content:

1. Determination of dissociation constants by measuring conductivity of weak acids
2. Determination of weak acids' dissociation constant via potentiometric titration

Semester-IV

Theoretical Papers (For Each, Full Marks: 50; Credit: 4)

MSCCHEMC401: Advanced Analytical Chemistry General

Course objective: To study the stability of complex and to determine the composition and stability constant of complex by different methods. To familiar with the basic principles and applications of different advanced spectroscopic methods such as heteronuclear NMR spectroscopy, CD/ORD, EPR, photoelectron spectroscopy, etc. To understand the basic principles of different electrochemical methods used in different analytical methods such as cyclic voltammetry, differential pulse voltammetry, coulometry, electrogravimetry, LSV and to familiar with batteries. To study the applications of radioisotopes in the field of analytical chemistry and pharmaceuticals. To study the effect of radiation in biological field.

Course outcome: To the end of this course the learners are able to evaluate the composition and stability constant of complex by different methods. Learner can explain different spectroscopic data and characterize different compounds by different spectroscopic methods such as NMR, CD/ORD, EPR, photoelectron spectroscopy, etc. Learners able to explain CV, coulometry, LSV curve and understand the working principles of batteries. Understand the different radioanalytical techniques and applications of different radio-isotopes for the treatment of different diseases. Became familiar with the biological effects of radiation.

Unit I

1. Complexes in aqueous solution (09 lectures)

pH-potentiometric, spectrophotometric methods (slope-ratio, mole-ratio and Job's method of continuous variation of measuring stability constants of complexes, Bjerrum half n method, stability of mixed ligand complexes and calculations; determination of composition, evaluation of thermodynamic parameters, factors influencing the stability of complexes

2. Advanced spectroscopic methods including hyphenated ones (16 lectures)

Instrumentation, presentation of spectra, Applications of heteronuclear NMR spectroscopy; ^{11}B, ^{13}C, ^{14}N, ^{17}O, ^{19}F and ^{31}P-NMR, ^{195}Pt. CD/ORD: methods, molecular dissymmetry and chiroptical properties, Cotton effect, Faraday effect in magnetic circular dichroism (MCD) and application. EPR: anisotropy, intensity, hyperfine spliting, Kramer's theorem, photoelectron spectroscopy, ESCA, UPS, Auger, AES, XRF and EXFAS; Synergistic benefit: spectroscopic and other tools in structure elucidation

Unit II

3. Electroanalytical methods II (09 lecturers)

Instrumentation: cyclic voltammetry, differential pulse voltammetry, coulometry, electrogravimetry, LSV; methods, low-temperature accessory, interfacing, conjunctive study, switching potential, electrode potential, pathways of electron transfer: EEE, EC, EC', ECE; electro-induced reactions; conventional secondary batteries: Ni-Cd, Ni-Fe, Ag-Zn, ZEBRA system; surface-modified study, materials preparation

4. Application of radiotracers and radiopharmaceuticals (09 lectures)

Radiotracers: isotope dilution; DIDA, IIDA and substoichiometric methods of analysis, application, nuclear activation analysis: principles, classifications and methods of nuclear activation analysis; special types of derivative activation analysis, depth profile activation analysis, cyclic activation analysis, charged-particle activation analysis (CPAA): PGNAA, PIXE, PIGE, IPAA, RBS; general considerations and factors; biosynthesis, factors in labeling: efficiency, isotope effect, specific methods of labeling

Radiopharmaceuticals: design of a new radiopharmaceutical: nuclear pharmacy: concept, pharmaceuticals and radiopharmaceuticals; radionuclide generators; ideal radiopharmaceuticals, methods of radiolabelling, specific radiopharmaceuticals for diagnostic and therapeutic purposes

5. Chemical and biological effects of radiation (07 lectures)

Ionizing radiation and its physical and chemical effect in target, water, radiolysis; definition of different units in radiation chemistry, calculation of radiation dose, biological effects, source of human data, lethal dose, permissible level of radiation dose; primary radiological products of water and their characterization, dosimetric concepts and quantities, thermoluminescence and lyoluminescence

Suggested books

R. M. Smith and A. F. Martell, *Critical Stability Constants*, 6 Vols, Plenum Press, New York, 1974-89.

M. Meloun, J. Havel and E. Hogfeldt, *Computation of Solution Equilibria: A Guide to Methods in Potentiometry, Extraction and Spectrophotometry*, Halsted, New York, 1988.

A. E. Martell and R. J. Motekaitis, *Determination and use of Stability Constants*, 2nd Edn, VCH, New York, 1992.

J. G. Grasselli, M. K. Snavely and B. J. Bulkin, *Chemical Application of Raman Spectroscopy*, Wiley, New York, 1981.

W. Kemp, *NMR in Chemistry: A Multinuclear Approach*, Macmillan Press, Hong Kong, 1986.

R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.

C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1994.

J. M. Hollas, *Modern Spectroscopy*, Wiley, New York, 1996.

K. Nakanishi and N. Berova, *Circular Dichroism,Principles and Applications*, VCH, New York, 1994.

H. Gunther, *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, Wiley, New York, 1995.

J. A. Iggo, *NMR Spectroscopy in Inorganic Chemistry* (Oxford Chemistry Primers), 2003.

A. K Brisdon, *Inorganic Spectroscopic Methods* (Oxford Chemistry Primers), Oxford University Press, (Indian Edn), 2005.

L. Kevan and R. N. Schwartz (Eds), *Time Domain Electron Spin Resonance*, John Wiley, New York, 1979.

J. E. Wertz and J. R. Boulton, *Electron Spin Resonance: Elementary Theory and Practical Applications*, Chapman and Hall, London, 1986.

N. M. Atherton, *Principles of Electron Spin Resonance*, Ellis Horwood/Prentice-Hall, Hemel Hempsted, 1993.

D. W. Turner, C. Baker and C. R. Bundle, *Molecular Photoelectron Spectroscopy*, Wiley Interscience, New York, 1970.

J. H. D Eland, *Photoelectron Spectra*, Butterworth, London, 1984.

T. L. Barr, *Modern ESCA: the Principles and Practice of X-ray Photoelectron Spectroscopy*, CRC Press, Boca Raton, FL, 1994.

D. P. Woodruff and T. A. Delchar, *Modern Techniques of Surface Science*, Cambridge University Press, Cambridge, 1988.

T. Thomson, M. D. Baker, A. Christie and J. F. Tyson, *Auger Electron Spectroscopy*, John Wiley, New York, 1985.

G.A. Ozin, A. C. Arsenault and L. Cadematiri, *Nanochemistry: A Chemical approach to Nanomaterrials*, Royal Society of Chemistry, London, 2009.

V. I. Goldanskii and R. H. Herber, *Chemical Applications of Mossbauer Spectroscopoy*, Academic Press, New York, 1968.

N. N. Greenwood and T. C. Gibb, *Mossbauer Spectroscopy*, Chapman and Hall, London, 1971.

R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.

J. M. Hollas, *Modern Spectroscopy*, Wiley, New York, 1996.

D. R. Crow, *Polarography of Metal Complexes*, Academic Press, London, 1979.

A. J. Bard and L. F. Faulkner, *Electrochemical Methods – Fundamentals and Applications*, 2nd Edn, Wiley, New York, 1998.

S. Torii, *Electro-Organic Syntheses*, Part I: *Oxidations*, Part II: *Reductions*, VCH, Weinheim, 1985.

D. E. Kyriacou and D. A. Jannakoudis, *Electrocatalysis for Organic Synthesis*, Wiley, New York, 1986.

J. Goodisman, *Electrochemistry: Theoretical Foundations*, Wiley, New York, 1987.

R. J. Gale (Ed), *Spectroelectrochemistry: Theory and Practice*, Plenum Press, New York, 1988.

J. Janata, *Principles of Chemical Sensors*, Plenum Press, New York, 1989.

J. O'M. Bockris and S. U. M. Khan, *Surface Electrochemistry*, Plenum Press, New York, 1993.

C. M. A. Brett and A. M. O. Brett, *Electrochemistry: Principles, Methods and Applications*, Oxford University Press, Oxford, 1993.

K. V. Kordesch, *Fuel Cells and Their Applications*, VCH, Weinheim, 1994.

D. T. Sawyer, A. Sobkowiak and J. L. Roberts, Jr, *Experimental Electrochemistry for Chemists*, 2nd Edn, Wiley, New York, 1995.

P. G. Bruce, *Solid-state Electrochemistry*, Cambridge University Press, Cambridge, 1995.

W. Schmickler, *Interfacial Electrochemistry*, Oxford University Press, Oxford, 1996.

C. A. Vincent and B. Scrosati, *Modern Batteries*, 2nd Edn, Arnold, London, 1997.

C. H. Hamann, A. Hamnett and W. Vielstich, *Electrochemistry*, Wiley-VCH, Weinheim, Germany, 2007.

J. W. T. Spinks and R. J. Woods, *An Introduction to Radiation Chemistry*, Wiley, New York, 1964.

J. F. Duncan and G. B. Cook. *Isotopes in Chemistry*, Clarendon Press, Oxford, 1968.

S. Ahrland, J. O. Liljerzin and J. Rydberg, *Chemistry of the Actinides*, Pergamon Press, Oxford, 1986.

W. D. Ehmann and D. E. Vance, *Radiochemistry and Nuclear Methods of Analysis*, John Wiley, New York, 1991.

J. Turner, *Atoms, Radiation and Radiation Protection*, Willey Interscience, New York, 1995.

Major Electives (any one from 0402-0407 and any one from 0405-0407)

MSCCHEMMJE401: Inorganic Chemistry Major II

Course objectives

- To understand the concepts and methods of electrochemical studies
- To understand the concepts of electron transfer
- To understand the concepts of inorganic photochemistry
- To understand the concepts of inorganic reaction reaction mechanism

Learning outcomes After completing the course the student will be expected to be able to:

- Acquire basic concepts of electrochemistry, electron transfer, inorganic photochemistry and reaction mechanism

Unit I

1. Electrochemical studies of redox non-innocent ligands and metal complexes (18 lectures)

Fundamentals, experimental findings of CV, DPV and coulometry, delving reversible, quasireversible and irreversible electrochemical and chemical processes in model compounds; electro-induced reactions: protic/electroprotic equilibrium, electrocatalysis, electropolymerisation, electrocrystallisation, electrochemiluminiscence; electrosynthesis, evaluating comproportionation constant, photoelectrochemistry, spectroelectrochemistry, excimer and its structure, excited state potential and chemical simulation, redox orbital, redox series, redox isomer, electron hopping, spatially isolated orbital; synergistic experiments and exposing electron transfer site, model case correlating biological processes

2. Mechanism of electron transfer reactions (07 lectures)

Fundamentals, complementary and non-complementary redox reactions, outer-sphere reaction, inner-sphere reaction, effect of bridging ligand in inner-sphere reaction, kinetics and mechanism, electron tunneling hypothesis, heteronuclear redox reaction and simplified Marcus theory; Marcus cross relationship and its application, remote attack, doubly-bridged process, ligand exchange, intervalence electron transfer, induced reaction, electron transport in biological systems and their simulations

Unit II

3. Inorganic photochemistry (13 lectures)

Preamble, photoexcitation, fluorescence, phosphorescence, photosensitization, quenching, charge and energy transfer, prompt and delayed reactions, excimer structure, substitution, fragmentation, isomerisation, exchange and redox reactions; chemiluminescence, photochromism; chemical actinometry and determination of quantum yield, inorganic photochemistry in biological processes and their model studies; applications of photochemical reactions of coordination compounds - synthesis and catalysis, solar energy conversion and storage

4. Inorganic and organometallic reaction mechanism (12 lectures)

Substitution reactions in square planar, tetrahedral and octahedral geometries with special reference to d^n ion complexes: operational tests, aquation and anation, reactions without metal-ligand bond breaking, kinetics of chelate formation, reaction mechanisms of organometallic systems, studies on fast reactions, kinetic and activation parameters - tools to propose a plausible mechanism; stereochemical changes: types of ligand rearrangements, isomerism in 4-, 5- and 6-coordinated complexes; reactions of coordinated ligands: model choice of metal and ligand, acid-base reaction, hydrolysis of esters, amides and peptides, aldol condensation, trans-amination, template reactions, organic synthesis with special reference to macrocyclic ligand; variable-temperature reactions in fluxional organometallic compounds

Suggested books

A. J. Bard, R. Parsons and J. Jordan, *Standard Potentials in Aqueous Solution*, Dekker, New York, 1985.
S. Torii, *Electro-Organic Syntheses*, Part I: *Oxidations*, Part II: *Reductions*, VCH, Weinheim, 1985.
D. E. Kyriacou and D. A. Jannakoudis, *Electrocatalysis for Organic Synthesis*, Wiley, New York, 1986.
J. Goodisman, *Electrochemistry: Theoretical Foundations*, Wiley, New York, 1987.
R. J. Gale (Ed), *Spectroelectrochemistry: Theory and Practice*, Plenum Press, New York, 1988.
J. Janata, *Principles of Chemical Sensors*, Plenum Press, New York, 1989.
J. O'M. Bockris and S. U. M. Khan, *Surface Electrochemistry*, Plenum Press, New York, 1993.
C. M. A. Brett and A. M. O. Brett, *Electrochemistry: Principles, Methods and Applications*, Oxford University Press, Oxford, 1993.
K. V. Kordesch, *Fuel Cells and Their Applications*, VCH, Weinheim, 1994.

D. T. Sawyer, A. Sobkowiak and J. L. Roberts, Jr, *Experimental Electrochemistry for Chemists*, 2nd Edn, Wiley, New York, 1995.

P. G. Bruce, *Solid-state Electrochemistry*, Cambridge University Press, Cambridge, 1995.

W. Schmickler, *Interfacial Electrochemistry*, Oxford University Press, Oxford, 1996.

C. A. Vincent and B. Scrosati, *Modern Batteries*, 2nd Edn, Arnold, London, 1997.

A. J. Bard and L. F. Faulkner, *Electrochemical Methods – Fundamentals and Applications*, 2nd Edn, Wiley, New York, 1998.

C. H. Hamann, A. Hamnett and W. Vielstich, *Electrochemistry*, Wiley-VCH, Weinheim, Germany, 2007.

W. L. Reynolds and R. W. Lumry, *Mechanism of Electron Transfer*, Ronald Press, New York, 1966.

H. Taube, *Electron Transfer Reaction of Complex Ions in Solution,* Academic Press, New York, 1970.

P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Shriver & Atkins Inorganic Chemistry,* 4th Edn, Oxford, 2006.

G. L. Miessler and D. A. Tarr, *Inorganic Chemistry,* 3rd Edn, Pearson, New Delhi, 2009.

B. N. Figgis, *Introduction to Ligand Field Theory*, Interscience, New York, 1966.

C. J. Ballhausen, *Molecular Electronic Structure of Transition Metal Complexes*, McGraw-Hill, London, 1979.

V. Balzani and V. Carassiti, *Photochemistry of Coordination Compounds,* Academic Press, New York, 1970.

A. W. Adamson and P. D. Fleischauer (Ed), *Concept of Inorganic Photochemistry*, Wiley, New York, 1975.

G. L. Geoffroy and M. S. Wrighton, *Organometallic Photochemistry*, Academic Press, New York, 1970.

D. Rendell and D. Mowthrope, *Fluorescence and Phosphorescence Spectroscopy*, John Wiley, New York, 1987.

C. E. Wayne and R. P. Wayne, *Photochemistry,* Oxford University Press, 1st Indian Edn, New Delhi, 2005.

J. R. Lakowicz, *Principles of fluorescence spectroscopy*, 3rd Edn, Springer, USA, 2006.

M. sauer, J. Hofkens and J. Enderlein, *Handbook of Fluorescence Spectroscopy and Imaging: from Singles to Ensembles*, Wiley-VCH, Weinheim, Germany, 2011.

F. Basolo and R. G. Pearson, *Mechanism of Inorganic Reactions*, 2nd Edn, Wiley, New York, 1967.

D. Katakis and G. Gordon, *Mechanisms of Inorganic Reactions*, John Wiley & Sons, New York, 1987.

R. G. Wilkinns, *Kinetics and Mechanism of Reactions of Transition Metal Complexes*, 2nd Edn, VCH, Weinheim, 1991.

R. B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems*, Oxford University Press, Oxford, 1998.

J. D. Atwood, *Inorganic and Organometallic Reaction Mechanisms*, 2nd Edn, Wiley-VCH, Weinheim, 1997.

S. Asperger, *Chemical Kinetics and Inorganic Reaction Mechanisms,* 2nd Edn, Springer, London, 2012.

MSCCHEMMJE402: Organic Chemistry Major II

Course Objectives: Teaches the chemistry involved in various photochemical reactions & their basic principles which enables students to learn a variety of photochemical reactions, their mechanisms; to understand and explain photochemical and photophysical processes and their quantum yield expressions, understanding the selection rules for electronic transitions and develop quantum mechanical formulation of Franck-Condon principle, to understand and explain the properties of electronically excited molecules, to understand and explain the nonradiative intramolecular electronic transitions, very scoring chapter from competitive point of view.

Teaches the chemistry involved in various advanced techniques in organic synthesis such as application of microwave irradiation, ultrasound and visible light irradiation, ball-milling, etc, to synthesize complex molecules with good yields.

Teaches the chemistry involved in various types of bio-polymers such as carbohydrates, proteins, nucleic acids, lipids, etc.

Learning Outcomes: After completing the chapter photochemistry, the student will be expected to be able to:
Explain fundamentals of photochemistry and the laws governing it.
Explain Jablonski diagram and describe and radiative and non-radiative transitions.
Describe photophysical kinetics of unimolecular and bimolecular processes.
Determine life time, redox potential, dipole moment, pK values, etc. of electronically excited molecules.

After completing the course, the student will be expected to be able to describe composition of biomolecules like proteins, nucleic acids, RNA and DNA, enzymes etc.

After completing the course, the student will be expected to be able to describe:
Conformational analysis of monosaccharides (pentoses and hexoses) and relative instability ratings;
Anomeric effect, mutarotation and abnormal mutarotation;
Structure of dsacchharides-sucrose and maltose.
General treatment of polysaccharide chemistry: isolation, purification, hydrolysis, methylation and periodic oxidation, Smith degradation, Barry degradation.

Unit I

1. Advanced techniques in organic synthesis (17 lectures)

Recent advances in organic synthesis focusing on the successful application of microwave (MW) irradiation, ultrasound (US)irradiation, visible light, ball-milling, and syntheses under solid-phase, room-temperature synthesis (ambient conditions)

2. Organic photochemistry II (8 lectures)

Photochemistry of arenes; photoreaction in solid state; method of generation and detection (ESR), radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, synthetic applications; cyclization of radicals; photo-induced oxidations and reductions

Unit II

3. Structure-function relationship in carbohydrates, proteins, lipids, nucleic acids and enzymes (18 lectures)

Carbohydrates: Basic structure and type of sugars, reactions, protection and deprotection, deoxy-sugars, amino sugars, glycal sugars and their synthetic aspects, mutarotaions, carbohydrates as chiral pools in organic synthesis; *Proteins*: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing, secondary structure of proteins, Ramachandran Diagram, forces responsible for holding of secondary structures, α-helix, β-sheets,tertiary structure of protein-folding, quaternary structure, biosynthesis of peptide chain;*Lipids*: Fatty acids, structure and function of triacylglycerols, glycerophospholipids,properties of lipid bi-layers, biological membranes, fluid mosaic model of membrane structure; *Nucleic acids*: Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding,structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it; *Enzymes*: Chemical and biological catalysis, properties of enzymes like catalytic power, specificity and regulation, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis; mechanism of enzyme action: transition state theory,examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease

4. Co-enzyme chemistry (07 lectures)

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes, Structure and biological functions for pyridoxal phosphate, NAD+, NADP+, FMN, FAD;mechanisms of reactions catalyzed by the above cofactors

Suggested books

D. Bogdal, *Microwave-assisted Organic Synthesis*, Elsevier, 2005.

G. Brahmachari, Room Temperature Organic Synthesis, Elsevier, 2015.

G. Brahmachari, *Green Synthetic Approaches for Biologically Relevant Heterocycles*, Elsevier, 2014.

A. Stolle and B. C. Ranu, *Ball Milling Towards Green Synthesis: Applications, Projects, Challenges*, Royal Society of Chemistry, 2014.

R. Cella,and H. A. Stefani, *Ultrasonic Reactions, In: Green Techniques for Organic Synthesis and Medicinal Chemistry* (eds W. Zhang and B. W. Cue), John Wiley & Sons, Ltd, Chichester, UK, 2012.

K. Tanka, Solvent-free Organic Synthesis, 2ndEdn., Wiley-VCH, 2009.

V. K. Ahluwalia and M. Kidwai,*New Trends in Green Chemistry*, Springer, 2004.

N. J. Turro,*Modern Molecular Photochemistry*, The Benjamin/ Cummings Publishing Co., Inc., 1978.

R. B. Woodward and R. Hoffman, *The Conservation of Orbital Symmetry*, Academic Press, 1970.

J.M. Coxon and B.H. Halton, *Organic Photochemistry*, Cambridge University Press, 1974.

S. Sankararaman,*Pericyclic Reactions – A Textbook*, Wiley-VCH Verlag, 2005.

M. Klessinger and J. Michl, *Excited States and Photo-Chemistry of Organic Molecules,* Wiley, 1995.

S. V. Bhat, B. A. Nagasampagi and M. Sivakumar, *Chemistry of Natural Products*, Narosa Publishing House, New Delhi, 2005.

X.-T. Liang and W.-S. Fang, *Medicinal Chemistry of Bioactive Natural Products*, John Wiley & Sons, 2006.

T. Hudlicky and J. W. Reed, *The Way of Synthesis*, Wiley-VCH, 2007.

H. Osbon, *Carvbohydrates*, Academic Press, 2003.

I. L. Finar, *Organic Chemistry, Volume 2: Stereochemistry And The Chemistry Natural Products*, 5thedn., Pearson Education India, 1956.

G. C. Howard and W. E. Brown, *Modern Protein Chemistry: Practical Aspects*, CRC Press, 2001.

S. P. Bhutani, *Chemistry of Biomolecules*, CRC Press, 2010.

O. Stone, *Chemical Biology: An Overview on Chemistry and Biology of the Biomolecules*, Foster Academics, 2015.

T. Palmer, *Enzymes: Biochemistry, Biotechnology and Clinical Chemistry*, Horwood, 2001.

T. D. H. Bugg, *Introduction to Enzyme and Coenzyme Chemistry, 3rd Edition*, Wiley, 2012.

MSCCHEMMJE403: Physical Chemistry Major II

Objectives: This chapter essentially deals with a major part of exactly solvable quantum mechanical problems. The analytical solutions of these problems involves the learning of some major mathematical techniques (e.g. Dirac's number operator formalism) frequently used in other parts of theoretical chemistry.

* To understand concept of force and fluxes.
* To understand chemistry of irreversible processes.

To introduce theories on molecular magnetism which is a interdisciplinary area including chemistry, physics and materials science that deals with the design, the synthesis, and the characterization of molecular based magnetic materials. It is not limited to this, however, and it is actually extended to every magnetic material that can be obtained by using molecular approaches. In this study we focus on the origin and development of the research in the field of molecular magnetism

Outcome: This chapter is aimed at building up the underlying basic concepts of various chemical ideas used in theoretical as well as in experimental chemistry. Thus the instructor thinks that this chapter has huge applicability in future research aspect. Students also get considerable amount of questions in various competitive examinations like GET/NET/ SET etc. from this chapter.

After completing the course the student will be expected to be able to:

• explain and determine entropy production in irreversible processes.

• apply Le Chateliar's principle on stationary states.

The students will acquire knowledge of (i) Interpretation of the electronic and magnetic properties. (ii) deals with problems on electron exchange and double exchange or spin crossover in small transition metal complexes, from mono- to di- and tetranuclear species, to the current investigations about magnetic anisotropy and spin dynamics or quantum coherence of simple mono- or large polynuclear complexes, (iii) potential applications in information data storage and processing in their further studies.

Unit I

1. Quantum mechanics of many electron systems (18 lectures)

Introduction to spin. Operator algebra for spin. Construction of matrix representation of spin operators, eigen values and eigen functions of spin operators. Many-electron wave functions- examples with 2 and 3 electron systems, Slater determinants. The Pauli exclusion principle. The Born-Oppenheimer approximation, Hartree self consistent field method, Koopman's theorem, Hartree-Fock method for many-electron systems. Coulomb operators, Exchange operators, Coulomb and Fermi hole, Restricted and unrestricted Hartree-Fock calculations, The Roothan equation. Correlation energy, Basis sets for electronic structure calculations. Spin-orbit interaction, The Condon-Slater rules. The Huckel and Extended Huckel MO method, Introduction to density functional theory, Definition of density, Hohenberg-Kohn variation theorem, Kohn-Sham equations, Exchange-correlation energy, Local density approximation, Generalized gradient approximation

2. Molecular interactions

(07 lectures)

Hamiltonian in absence and presence of external fields, forces in molecules, Hellmann-Feynmann theorem, perturbative treatment of electric polarisability, intermolecular interaction - calculation of dispersion energy, the London formula

Unit II

3. Irreversible thermodynamics and introductory course on non-equilibrium statistical mechanics
(18 lectures)

Thermodynamic criteria for Non-equilibrium states. Entropy production in irreversible process. Entropy balance equations. Generalized flux and forces.Stationary states.Coupling of irreversible process, Phenomenological equations.Microscopic reversibility and Onsager equation.Applications in physico-chemical and biological phenomena.

Einstein's theory of Brownian motion, Langevin description of Brownian motion: general expression for mean square displacement (i) short time limit and (ii) long time limit. Fluctuation-dissipation relation, Fokker-Planck equation, Brownian motion in phase space (motion in a force field): Kramers' equation. Application to Kramer's theory and transport problems, Master equations and its applications.

4. Electric and magnetic properties of molecules

(07 lectures)

Dielectric polarization; Debye equation and its limitation; Onsager's reaction field model; electric polarizability of molecules; magnetic susceptibility - diamagnetic and paramagnetic, Currie law

Suggested books

A. Szabo, N. S. Ostlund, Modern Quantum Chemistry, Dover Publications, Inc, NY

P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.

L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, New York, 1985.

A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi, 1989.

F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, New Delhi, 1990.

D. A. McQuarrie, *Quantum Chemistry,* Viva Books Pvt Ltd, New Delhi, 2003.

I. N. Levine, Quantum Chemistry, PHI Learning Pvt. Ltd, New Delhi, 2010.

E. Merzbacher, Quantum Mechanics, Wiley, 1998.

A. J. Stone, *The Theory of Intermolecular Forces*, Clarendon Press, Oxford, 1996.
C. J. F. Böttcher, *Theory of Electric Polarisation*, Vols 1 and 2, Elsevier Scientific Publishing Co, New York, 1973.
D. W. Davies, *The Electric and Magnetic Properties of Molecules*,
I. Prigogine, *Introduction to Thermodynamics of Irreversible Processes*, Inter science Publishers, 1967.
R. Zwanzig, Nonequilibrium Statistical Mechanics, Oxford University Press.

MSCCHEMMJE404: Inorganic Chemistry Major III

Course Objective: To impart knowledge of different types of supramolecules, structures and their applications as organic-inorganic materials, sensors, and devices. In particular, supramolecular chemistry is focused on understanding the physics of noncovalent bonding. Teaches the chemistry/mechanism of action of various commercially available antibiotics and life saving drugs

Outcome: The students will acquire knowledge of (i) details of synthesis, structure as well as reaction of supramolecules, (ii) Molecular recognition and nature of bindings involved in biological systems (iii) Structure of supramolecules of various types in solid state (iv) Applications of supramolecules in miniaturization of molecular devices.

Unit I

1. Supramolecular chemistry II (12 lectures)

Judicious choice of geometry setter/blocker/spacer/counter ion – an essential prerequisite, hydrogen bonding, π…π, C-H…π, halogen…π, S…π, etc interactions, allosterism, proton and hydride sponges, principle of three C's, lock and key principle, host-guest interaction, self organization and self complementarity, receptors, superstructures in inorganic, metallo-organic and organometallic compounds, 0D, 1D, 2D, 3D architectures and hierarchies, supramolecular devices

2. Inorganic materials (13 lectures)

Molecules and crystals to materials, art of synthesis, predictable crystalline architecture, intermolecular and interion interactions, secondary building unit (SBU), surface functionalisation, hysteresis, robust and directional interactions, click chemistry, functional materials: conducting, superconducting, magnetic, non-linear, porous, luminous, liquid crystals, quantum dots, catalysts, molecular and electronic devices, biosensors, biomineralization, proteomics, dendrimers, molecular recognition

Unit II

3. Molecular magnetism II (13 lectures)

Isolation of different molecular magnets, magnetic interactions in di- and polynuclear systems and clusters, cryogenic experiment, mechanism of exchange interaction, Bleaney-Bowers equation, antiferromagnetism (AF), ferromagnetism (F), single molecule magnet, deliberate synthetic approach of ferromagnetically coupled system, accidental orthogonality, spin canting, canted-AF, canted-F, spin frustration, admixed-spin, spinflop, metamagnetism, superparamagnetism, long-range ordering, calculation of ground state and spin manifold, magnetization versus field studies, inorganic, organic, metal-organic and organometallic magnetic materials

4. Structure-function relationship (12 lectures)

A sheer necessity and an ultimatum, thermodynamic and kinetic parameters; diagnostic probes: spectroscopic, thermal, electrochemical, magnetic, crystallographic; parameters: stretching frequency, chemical shift, spin-spin coupling constant, isomer shift, potential value, bond distance, bond angle, torsion angle, crystal packing and Madelung constant, magnetic moment value, rate constant, half life, correlation diagram, room temperature and variable-temperature results, breakthrough and legacy

Suggested books

F. Vogtle, *Supramolecular Chemistry: An Introduction*, Wiley, Chichester, 1991.

B. Dietrich, P. Viout and J. -M. Lehn, *Macrocyclic Chemistry – Aspects of Organic and Inorganic Supramolecular Chemistry*, VCH, Weinheim, 1993.

J. -M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, VCH, Weinheim, 1995.

G. R. Newkome, C. N. Moorefield and F. Vogtle, *Dendritic Molecules*, VCH, Weinheim, 1996.

G. A. Jeffrey, *An Introduction to Hydrogen Bonding,* Oxford University Press, Oxford, 1997.

S. T. Hyde, B. Ninham, S. Anderson, Z. Blum, T. Landh, K. Larsson and S. Liddin, *The Language of Shape*, Elsevier, Amsterdam, 1997.

G. R. Desiraju (Ed), *Crystal Design: Structure and Function, Perspectives in Supramolecular Chemistry*, Vol 7, Wiley, Chichester, 2003.

J. W. Steed and J. L. Atwood,*Supramolecular Chemistry*, 2nd Edn, John Wiley & Sons, New York, 2009.

K. Rurack and R. Martinez-Manez (Eds), *The Supramolecular Chemistry of Organic-Inorganic Hybrid Materials,* John Wiley & Sons, Hoboken, New Jersey, 2010.

R. Xu, W. Pang and Q. Huo (Eds), *Modern Inorganic Synthetic Chemistry*, Elsevier, New York, 2011.

E. R. T. Tiekink and J. Zukerman-Schpector (Eds), *The Importance of Pi-Interactions in Crystal Engineering: Frontiers in Crystal Engineering*, 1st Edn, John Wiley & Sons, Chichester, UK, 2012.

V. Balzani and F. Scandola, *Supramolecular Photochemistry*, Ellis Horwood, Chichester, 1991.

U. Schubert and N. Hüsing, *Synthesis of Inorganic Material*, Wiley-VCH, Weinheim, 2004.

C. N. R. Rao, A. Muller and A. K. Cheetham, *The Chemistry of Nanomaterials: Synthesis Properties and Applications*, Wiley-VCH, Weinheim, Germany, 2004.

G. A. Ozin and A. C. Arsenault, *Nanochemistry: A Chemical Approach to Nanomaterials*, RSC Publishing, Cambridge, 2005.

C. N. R. Rao, A. Muller and A. K. Cheetham, *Nanomaterials Chemistry: Recent Developments and New Directions*, Wiley-VCH, Weinheim, Germany, 2007.

E. Ruiz-Hitzky, K. Ariga and Y. Lvov, *Bio-inorganic Hybrid Nanomaterials. Strategies, Syntheses, Characterization and Applications*, Wiley-VCH, Weinheim, 2008.

A. Sayari and M. Jaroniec, *Nanoporous Materials*, World Scientific Publishing, Singapore, 2008.

L. Cademartiri and G. A. Ozin, *Concepts of Nanochemistry*, Wiley-VCH, Weinheim, 2009.

J. N. Lalena, D. A. Cleary, E. E. Carpenter and N. F. Dean, *Inorganic Materials Synthesis and Fabrication*, John Wiley & Sons, Inc. Hoboken, New Jersey, 2008.

P. Comba, T. W. Hambley and B. Martin, *Molecular Modeling of Inorganic Compounds*, 3rd Edn, Wiley-VCH, Weinheim, 2009.
S. R. Batten, S. M. Neville and D. R. Turner, *Coordination Polymers Design, Analysis and Application*, The Royal Society of Chemistry, Cambridge, 2009.
M. -C. Hong and L. Chen (Eds), *Design and Construction of Coordination Polymers*, John Wiley & Sons, Inc, Hoboken, New Jersey, 2009.
J. N. Lalena and D. A. Cleary, *Principles of Inorganic Materials Design*, 2nd Edn, John Wiley & Sons, Inc, Hoboken, New Jersey, 2010.
V. Balzani, A. Credi and M. Venturi,*Molecular Devices and Machines*, Wiley-VCH, Weinheim, 2003.
M. Petty,*Molecular Electronics: From Principles to Practice*, Wiley, Chichester, 2008.
L. R. Macgillivray (Ed), *Metal-Organic Frameworks: Design and Application*, John Wiley & Sons, Inc, Hoboken, New Jersey, 2010.
S. R. Marder, J. E. Sohn and G. D. Stucky (Eds), *Materials for Non-linear Optics: Chemical Perspectives,* ACS Symposium Ser, 1991.
R. W. Boyd, *Nonlinear Optics*, Academic Press, San Diego, 1992.
R. L. Carlin, *Magnetochemistry*, Springer-Verlag, New York, 1986.
O. Kahn, *Molecular Magnetism*, VCH, New York, 1993.
P. Day and A. E. Underhill (Eds), *Metal-organic and Organic Molecular Magnets*, RSC, London, 2000.
P. M. Lathi (Ed), *Magnetic Properties of Organic Materials*, Marcel Dekker, New York, 1999.
J. S. Miller and M. Drillon (Eds), *Magnetism: Molecules to Materials, V; Molecule-based Magnets*, Wiley-VCH, Weinheim, 2005.
P. Gutlich and H. A. Goodwin, *Spin Crossover in Transition Metal Compounds I*, Springer, Berlin, 2004.
F. E. Mabbs and D. J. Machin, *Magnetism and Transition Metal Complexes*, Dover Publications, 2008.
R. Winpenny (Ed), *Single-Molecule Magnets and Related Phenomena*, Structure and Bonding Series, Vol. 122, Springer, Berlin, 2010.
B. D. Cullity and C. D. Graham, *Introduction to Magnetic Materials,* 2nd Edn, John Wiley & Sons, New York, 2011.
K. H. J. Buschow, *Handbook of Magnetic materials,* Vol 20, Elsevier, New York, 2012.
D. Gatteschi, R Sessoli and J. Villain, *Molecular Nanomagnets*, Oxford University Press, Oxford, 2006.
R. Hilzinger and W. Rodewald, *Magnetic Materials*, Wiley, New York, 2013.
B. Pignataro (Ed), *Tomorrow's Chemistry Today – Concepts in Nanoscience, Organic Materials and Environmental Chemistry,* Wiley-VCH, Weinheim, 2008.
L. Cademartiri and G. A. Ozin, *Concepts of Nanochemistry,* Wiley-VCH, Weinheim, 2008.
B. R. Eggins, Chemical Sensors and Biosensors, Wiley India Pvt Ltd, New Delhi, 2002.
S. Chandrasekhar, *Liquid Crystals*, 2nd Edn, Cambridge University Press, Cambridge, 1992.
G. R. Desiraju, *Crystal Engineering: Designing of Organic Solids*, Elsevier, New York, 1989.
D. Braga, F. Grepioni and A. G. Orpen, *Crystal Engineering: from Molecules and Crystals to Materials*, Kluwer Academic Publishers, Dordrecht, 1999.
U. Schubert and N. Husing, *Synthesis of Inorganic Material*, 2nd Edn, Wiley-VCH Verlag GmbH& Co, Weinheim, 2005

X. -D. Xiang and I. Takenchi (Eds), *Combinatorial Synthesis,* Marcel Dekker, New York, 2003.
E. I. Stiefel (Ed), *Dithiolene Chemistry: Synthesis, properties, and Applications*, John Wiley & Sons, New Jersey, 2004.
P. Gomez-Romero and C. Sanchez (Eds), *Functional Hybrid Materials*, Wiley-VCH, Weinheim, 2004.
M. F. C. Ladd and R. A. Palmer, *Structural Determination by X-ray Crystallography*, 3rd Edn, Plenum, New York, 1994.
D. Farrusseng (Ed), *Metal-Organic Framework: Applications from Catalysis to Gas Storage*, Wiley-VCH, Verlag, GmbH& Co, 2011.

MSCCHEMMJE405: Organic Chemistry Major III

Course Objectives: To learn about various types of pericyclic reactions including cycloaddition, electrocyclic reactions and sigmatropic rearrangement.

To impart knowledge of different types of supramolecules, structures and their applications as organic-inorganic materials, sensors, and devices. In particular, supramolecular chemistry is focused on understanding the physics of noncovalent bonding.

Teaches the chemistry/mechanism of action of various commercially available antibiotics and life saving drugs.

To learn about various types of biosynthetic approach of biologically relevant natural products.

Learning Outcomes: After completing the chapter pericyclic reactions, the learners should be able distinguish mechanistic difference between a perycyclic and an ionic reactions. They should be able to design synthetic scheme of various commercial or non-commercial chemicals by using the concept of pericyclic reactions.

The students will acquire knowledge of (i) details of synthesis, structure as well as reaction of supramolecules, (ii) Molecular recognition and nature of bindings involved in biological systems (iii) Structure of supramolecules of various types in solid state (iv) Applications of supramolecules in miniaturization of molecular devices.

After completing the course, the student will be expected to be able to describe composition of biomolecules like proteins, nucleic acids, RNA and DNA, enzymes etc.

After completing the course, the student will be expected to be aware of mechanism of action of various antibiotics and life saving drugs.

After completing the course, the student will be expected to be able to describe biosynthetic approach of various biologically relevant natural products.

Unit I

1. Pericyclic reactions II (08 lectures)

Sigmatropic reactions: Definition, classification, stereochemistry, Woodward-Hoffmann rules, illustrations for [1,2]-, [1,3]-, [1,4]-, [1,5]-, [2,3]- and [3,3]-sigmatropic rearrangements, Claisen rearrangement, Cope rearrangement; Chelotropic reactions: Definition, Woodward-Hoffmann rules, examples of chelotropic reactions (chelotropic reactions involving SO_2, chelotropic extraction of nitrogen, chelotropic decarbonylation of ketones, chelotropic trapping of nitric oxide), synthetic applications; Ene reactions: Definition, classification, catalyzed and uncatalyzed ene reactions, stereochemistry of ene reactions – diastereoselection, oxy-ene and anionic oxy-ene-reactions, imino-ene reactions, carbonyl ene-reactions, singlet oxygen ene-reactions, retro-ene reactions.

2. Supramolecular chemistry (07 lectures)

Basic concepts of supramolecular chemistry, different non-covalent forces (hydrogenbonding, cation-π, CH-π, π-stacking, hydrophobic, hydrophilic interactions etc.)leading to strong bonding of guest molecules to the host, design principleof host or receptor molecules, different experimental techniques to characterize the host–guest complexation, example of molecular receptors: crown ethers, ionophores,cyclophanes, cyclodextrins and their application in specific recognition processes.

3. Antibiotics, antidiabetic and cardiovascular drugs: Chemical aspects (10 lectures)

Antibiotics: Cell wall biosynthesis, inhibitors, β-lactam rings, synthesis of penicillin;synthesis and mode of action of sulphonamides, nalidixic acid, norfloxacin, aminosalicyclic acid, ethinamide, fluconazole, chloroquin and premaquin; Antidiabetic drugs: insulinsensitizers (biguanides, thiazolidinediones), secretagogues (sulfonylureas, nonsulfonylurea secretagogues, alpha-glucosidase inhibitors, peptide analogues (injectable incretin mimetics, injectable amylin analogues); *Cardiovascular drugs*: Introduction to cardiovascular diseases, synthesis and mode of action of statins, amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil and methyl dopa

Unit II

4. Chemistry of polyphenolics (12 lectures)

Natural occurrence, chemical aspects, biological activities and therapeutic potential of some notable natural polyphenolics from the respective group: ellagitannins, flavonoindsand xanthonoides

5. Chemistry of steroidal hormones (07 lectures)

Chemistry and function of some steroidal hormones – estrogens, estrone, estradiol, estriol, progesterone, testosterone, oral contraceptives, anabolic steroids

6. Biosynthesis of some selected biologically relevant natural products (06 lectures)

Atropine, quinine, nicotine, abietic acid, β-carotene, cholesterol

Suggested books

T.L. Gilchrist and R.C. Storr, *Organic Reactions and Orbital Symmetry*, 2nd Edn., Cambridge University Press, 1979.

R. B. Woodward and R. Hoffman, *The Conservation of Orbital Symmetry*, Academic Press, 1970.

S. Sankararaman, *Pericyclic Reactions – A Textbook*, Wiley-VCH Verlag, 2005.

I. Fleming, *Pericyclic Reactions*, Oxford University Press, 1996.

F. Vögtle, *Supramolecular Chemistry: An Introduction*, John Wiley & Sons, 1991

J. M. Lehn, *Supramolecular Chemistry: Concept and Perspectives*, Wiley-VCH, 1995

P. J. Cragg, *Supramolecular Chemistry*, Springer, 2010.

H.-J. Schneider and A. Yatsimirsky, *Principles and Methods in Supramolecular Chemistry*, Wiley-VCH, 1999.

K. Ariga and T. Kunitake,*Supramolecular Chemistry - Fundamentals and Applications*, Springer, 2006.

J. C. Gallagher and C. MacDougall,*Antibiotics Simplified*, 3rd Revised edition, Jones and Bartlett Publishers, Inc. 2013.

C. Walsh, *Antibiotics: Actions, Origins, Resistance*, Wiley-VCH, 2016.

S. Sánchez and A. L. Demain, *Antibiotics: Current Innovations and Future Trends*,Caister Academic Press, 2015.

B. Testa and U. A. Meyer, *Antidiabetic Agents: Recent Advances in their Molecular and Clinical Pharmacology*,Acdemic Press, 1996.

K. Chatterjee and E. J. Topol, *Cardiac Drugs*, 1 edition,Jaypee Brothers Medical Pub., 2013.

W. H. Frishman and D. A. Sica, *Cardiovascular Pharmacotherapeutics - 3rd Edition*, CardioText, 2011.

Atta-ur-Rahman and M.I. Choudhary, *Frontiers in Cardiovascular Drug Discovery*, Bentham Publications, 2010.

S. Quideau, *Chemistry and Biology of Ellagitannins*, World Scientific Publishing Co., 2009.

O. M. Anderson and K. R. Markham, *Flavonoids: Chemistry, Biochemistry and Applications*, CRC Press, Taylor & Francis, 2006.

S. K. Talapatra and B. Talapatra, *Chemistry of Plant Natural Products*, Springer, 2012.

S. V. Bhat, B. A. Nagasampagi and M. Sivakumar, *Chemistry of Natural Products*, Narosa Publishing House, New Delhi, 2005.

M. M. M. Pinto, *Chemistry of Love and Sex*, Wiley-VCH, 2012.

D. B. Gower, *Steroid Hormones*, Year Book Medical Pub., 1979.

X.-T. Liang and W.-S. Fang, *Medicinal Chemistry of Bioactive Natural Products*, John Wiley & Sons, 2006.

P. Manitto, *Biosynthesis of Natural Products*, Ellis Horwood Ltd., 1981.

T. Hudlicky and J. W. Reed, *The Way of Synthesis*, Wiley-VCH, 2007.

MSCCHEMMJE406: Physical Chemistry Major III

Course objectives

* To understand theories of Molecular reaction dynamics.
* To understand theories of scattering of probes of the collision dynamics
* To understand potential energy surface in different dimension (2D and 3D), Imaginary frequency

To give Basic knowledge of bond and band concept from molecular orbital theory. To provide the concept of Brilloin zone, band gap, etc.

Classical and quantum mechanical concept of band theory, and their application with respect to electrical and thermal transport etc. Give a complete idea of semiconductors, p-n junction and superconductors etc.

* To explain the concept of photochemistry.

* To understand and explain photochemical and photophysical processes and their quantum yield expressions.

* To understand the selection rules for electronic transitions and develop quantum mechanical formulation of Franck-Condon principle.

* To understand and explain the properties of electronically excited molecules.

* To understand and explain the nonradiative intramolecular electronic transitions.

* To understand basic principles of LASER and application of LASER

* To understand concept of alternative source of renewable energy.

* To explore the nanohybrid materials efficient in the production of renewable energies..

Learning outcomes After completing the course the student will be expected to be able to:

• explain about molecular reaction dynamics

• derive rate expression in terms of atomic and molecular partition functions.

• explain various types of PES and the term imaginary frequency.

Students can gather a vast knowledge of band theory of solids, semiconductors and thermal and electrical transport mechanism.

To understand the band structure of non-transition and transition metal band and their subsequent properties. Concept of Hall effect to detect the type of semiconductor

After completing the course the student will be expected to be able to:

• explain fundamentals of photochemistry and the laws governing it.

• explain Jablonski diagram and describe and radiative and non- radiative transitions.

• describe photophysical kinetics of unimolecular and bimolecular processes.

• determine life time, redox potential, dipole moment, pK values, etc. of electronically excited molecules.

• describe Potential energy diagram for donor acceptor system and Polarized luminescence.

* know about the working mechanism of different kinds of laser and their diversified application into various fileds.

After completing the course the student will be expected to be able to:

• explain the term of alternative source of energy and how it can be regenerated and reused.

• apply Le Chateliar's principle on stationary states.

Unit I

1. Molecular reaction dynamics (MRD) (12 lectures)

Motivation for studying MRD, Spectator model, Molecular collisions, Vocabularies in MRD, Dynamics of elastic molecular collisions, Collision cross section, The impact parameter, Centrifugal energy and barrier, The reaction cross section, Reaction probability, opacity function, translation energy requirements of chemical reactions, Scattering as probe of the collision dynamics, The angular function, The deflection function, Scattering as a probe for the potential, Product angular distribution in reactive collisions, Potential energy surfaces (PES) for a reaction, attractive and repulsive PES. Polyani's rules

2. Solid state chemistry (13 lectures)

Crystal structure: lattice, basis, concept of Bravais lattice, primitive and non primitive cell for SC, BCC, FCC, HCP; construction of Wigner Seitz cell; different lattice structures: diamond, zincblande, etc.; crystallographic point group and space group Reciprocal lattice, relation with Miller indices; Fourier transformation and Fourier space, conversion of primitive axes, Brillouin zone for 1D, 2D and 3D lattices, Determination of crystal structure: Bragg's condition, von Laue condition, their interrelation, geometrical structure factor, Electronic structure: Classical Drude model and its limitation, DC electrical conductivity, equation of motion; Hall effect, concept of charge carrier, thermal conductivity; Sommerfeld theory, ground state properties of electron gas, Fermi energy, Fermi surface; thermal properties of metal, Electron level in periodic potential: Bloch's theorem and its consequences; weak periodic potential, density of states, band structure; interaction of bands, tight-binding formulations; semiconductor solids and their properties.

Unit II

3. Photochemistry and Laser principles

(15 lectures)

Excitation of molecules – Singlet and Triplet states. Jablonsky diagrams, Radiative and Non-radiative relaxations. Franck-Condon principle.Absorption, emission and excitation spectra - mirror symmetry. Florescence, Phosphorescence, quantum yield, mechanism and decay kinetics of photophysical process, quenching (dynamic and static), Stern-Volmer equation, Excited state processes – proton transfer, electron transfer and energy transfer (Forster's dipole coupling). Marcus Theory. Solvent effect in spectroscopy.Solvation dynamics.Non-linear optical processes. Stimulated emission of radiation.Principles of Laser action.Population inversion, Basic elements in laser, characteristics of laser radiation, Applications of Lasers.

4. Alternative Energy Studies (10 lectures)

Solar energy conversion, artificial photosynthesis; Si-p-n junction solar cell, basic principles and application, Dye-sensitized solar cells; structure, components and their functions. operating principles, Efficiencies of solar cells. Quantum dot sensitized solar cell, Nano hybrid materials for solar cell application.

Suggested books

R. D. Levine, Molecular Reaction Dynamics, 2006, Oxford University Press.

R. D. Levine, R. B. Bernstein, Molecular Reaction Dynamics and Chemical Reactivity, Oxford University Press, 1987.

C. Kittel, *Introduction to Solid State Physics*, 4th Edn, John Wiley & Sons, New York.

P. A. Cox, *The Electronic Structure & Chemistry of Solids*, Oxford University Press, Oxford, 1987.

A. R. West, Basic Solid State Chemistry, Wiley
L. Azzarof, Introduction to Solids, 1966
K, K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, New Age International Publishers.
N. J. Turro, Modern Molecular Photochemistry, University Science Books
B. O'Regan, M. Gratzel, Nature, Vol- 353, Page-737, 1991.
M. Gratzel, J. Photochemistry and Photobiology C, Photochemistry Reviews, Vol-4, Page-145, 2003.
U. Mehmood et al. Review article on Recent advances in dye sensitized solar cells, Advances in Materials Science and Engineering Volume 2014, Article ID 974782.

Major Elective Practical (any one) (For Each, Full Marks: 50; Credit: 4)

MSCCHEMMJE407: Inorganic Chemistry Major: Practical II

Learning objectives

* To acquire the ideas of coordination compounds synthesis using self assembly

* Knowledge of growing of single crystals

Learning Outcomes At the end of the course, the learners should be able to:

• explain the principle behind the experiments performed in the laboratory

Contents:

1. Preparation of inorganic and coordination compounds using self-assembly
2. Growing of single crystals
3. Spectral, thermal, electrochemical and magnetic studies
4. Reactivities
5. Kinetic and mechanistic studies of some selected reactions (substitution and redox)

MSCCHEMMJE408: Organic Chemistry Major: Practical II

Learning objectives

* To acquire the ideas of multi step organic synthesis

Learning Outcomes At the end of the course, the learners should be able to:

• explain the principle behind the experiments performed in the laboratory

Contents:

1. Preparation of organic compounds involving multiple step reactions
2. Characterization of organic compounds using spectroscopic methods

MSCCHEMMJE409: Physical Chemistry: Major II

Learning objectives

* To validate the conceptual understanding acquired from the theory classes.

* To perform experiments applying concepts of kinetics, charge transfer and host-guest interaction

* To know the basic principles TCSPC technique and how to operate to acquire data.

Learning Outcomes At the end of the course, the learners should be able to:

• explain the principle behind the experiments performed in the laboratory

• plan and perform experiments and interpret experimental results.

Contents:

1. Instrumental methods of studying hydrolysis, solubility and kinetics; elementary computer-based numerical methods
2. Study on charge transfer/EDA complexes
3. Determination of the binding constant of a 'Host-Guest' complex by spectrophotometric method
4. Determination of the thermodynamic parameters of the formation of a 'Host-Guest' complex
5. Fluorescence lifetime measurement
6. Study of a chemical oscillating system

Term Paper/Project work* (any one from 0411-0413)

(For Each, Full Marks: 50; Credit: 6)

MSCCHEMC402: Inorganic Chemistry Term Paper/Project

MSCCHEMC403: Organic Chemistry Term Paper/Project

MSCCHEMC404: Physical Chemistry Term Paper/Project

Course objectives

* To understand techniques followed in identifying research problem.

* To understand strategies in solving research problem.

Learning Outcomes At the end of the course, the learners should be able to:

• identify a research issue and frame methodology to solve it.

• write well organized report.

*In each discipline concerned MSCCHEMC402-404, topic-selection in consultation with the teacher; literature search from different reference books and using internet search; typed write-up with proper tables, structures, figures and literature to be submitted (approximately 25-30 pages with 12 font size); seminar lecture on this topic to be delivered in presence of all the teachers and an external subject expert