MASTER OF SCIENCE

IN

CHEMISTRY

(Regulations 2018)

CURRICULUM AND SYLLABUS

(For students admitted from academic year 2018-2019 onwards)

UNDER CHOICE BASED CREDIT SYSTEM

SRM
INSTITUTE OF SCIENCE & TECHNOLOGY
(Deemed to be University u/s 3 of UGC Act, 1956)

DEPARTMENT OF CHEMISTRY

SRM INSTITUTE OF SCIENCE AND TECHNOLOGY

SRM NAGAR, KATTANKULATHUR – 603 203

M.Sc. CHEMISTRY

(For students admitted from the academic year 2018-2019 onwards)

CURRICULUM AND SYLLABUS

Objectives:

1. To develop critical analysis and problem solving skills required in the application of principles of Chemistry.
2. To prepare students with a working knowledge of experimental techniques and instrumentation required to work independently in research or industrial environments.
3. To develop student strength in organizing and presenting acquired knowledge coherently both orally and in written discourse.
4. To prepare the students to successfully compete for current employment opportunities.

Eligibility:

B.Sc. Chemistry with Chemistry as a major subject, or Triple major subjects with Chemistry as one of the major subjects

Duration:

2 Years (4 Semesters).

STUDENT OUTCOMES

The curriculum and syllabus for the Master degree in Chemistry (2018-19) conform to outcome based teaching learning process. In general, TWELVE STUDENT OUTCOMES (a-l) have been identified and the curriculum and syllabus have been structured in such a way that each of the courses meets one or more of these outcomes. Student outcomes describe what students are expected to know and be able to do by the time of graduation. These relate to the skills, knowledge, and behaviours that students acquire as they progress through the program. Further each course in the program spells out clear instructional objectives which are mapped on to the student outcomes.

On successful completion of this Program, students will have the ability to

a. Acquire knowledge and understanding of essential facts, concepts, principles and theories relating to the subject areas identified.
b. Develop Skills to evaluate, analyse and interpret chemical information and data.
c. Solve problems competently by identifying the essential parts of a problem and formulating a strategy for solving the problem.
d. Use of computers and available software in data analysis.
e. Use standard laboratory equipments, modern instrumentation and classical techniques to carry out experiments.
f. Develop skills to interpret and explain the limits of accuracy of experimental data in terms of significance and underlying theory
g. Think creatively (divergent and convergent) to propose novel ideas in explaining facts and figures or providing new solutions to problems.
h. Function effectively on teams to accomplish a common goal
i. Understand the professional, ethical, legal, security and social issues and responsibilities
j. Communicate effectively with a range of audiences
k. Understand the best practices and standards in the field and their application
l. Assist in the creation of an effective project plan.

Contents

CURRICULUM

M.Sc. (Chemistry) **Total credits: 82**

As per UGC Regulation 2016 (Credit Framework for Online Learning Courses through SWAYAM), SRMIST strongly encourages the use of SWAYAM (Study Web of Active Learning by Young and Aspiring Minds) platform.

1. Students shall be allowed to choose one SWAYAM course per semester on the recommendation of the faculty advisor and the credits will be transferred.
2. Based on the curriculum, students shall be allowed to choose one major core course from SWAYAM.
3. Suitable courses available on SWAYAM can also be chosen as an elective (major/non-major).

SEMESTER I

Category	Course Code	Course	L	T	P	O	L+T+P	C
Major Core	18PCY101	Chemical Bonding, Molecular Geometry and Group Theory	3	1	-	1	4	4
	18PCY102	Classical and Statistical Thermodynamics	3	1	-	1	4	4
	18PCY103	Organic Chemistry I-Structure and Reactivity	3	1	-	1	4	4
	18PCY104	Main Group Elements and Nuclear Chemistry	3	1	-	1	4	4
	18PCY105	Physical Chemistry Laboratory	-	-	6	-	6	3
		Total	**12**	**4**	**6**	**4**	**22**	**19**

SEMESTER II

Category	Course Code	Course	L	T	P	O	L+T+P	C
Major Core	18PCY201	Quantum Chemistry and Molecular Spectroscopy	3	1	-	1	4	4
	18PCY202	Organic Chemistry II- Structure and Reactivity	3	1	-	1	4	4
	18PCY203	Advanced Transition Metal Chemistry	3	1	-	1	4	4
	18PCY204	Organic Chemistry Laboratory	-	-	6	-	6	3
	18PCY205	Inorganic Chemistry Laboratory	-	-	6	-	6	3

Category	Course Code	Course	L	T	P	O	L+T+P	C
	18PCY206	Seminar (Based on recent research articles)*	-	-	2	-	2	1
Non-major Elective I		Open Elective –I	2	-	-	-	2	2
Total			**12**	**3**	**12**	**3**	**28**	**21**

L – Lecture, T – Tutorial, P – Practical, O - Outside Class, C– Credits
Note:* Continuous assessment [Full Internal]

SEMESTER III

Category	Course Code	Course	L	T	P	O	L+T+P	C
Major Core	18PCY301	Organometallic and Bioinorganic Chemistry	3	1	-	1	4	4
	18PCY302	Chemical Kinetics and Surface Chemistry	3	1	-	1	4	4
	18PCY303	Advanced Organic Chemistry	3	1	-	1	4	4
	18PCY304	Project Phase I *(Research & Seminar)**	-	-	8		8	4
Major Elective I	18PCY3EA	Advanced Electrochemistry	3	1	-	1	4	4
	18PCY3EB	Heterocyclic Chemistry and Total Synthesis ofNatural Products						
	18PCY3EC	Polymer Science						
Non-major Elective II		Open Elective –II	2	-	-	-	2	2
Total			**14**	**4**	**8**	**4**	**26**	**22**

SEMESTER IV

Category	Course Code	Course	L	T	P	O	L+T+P	C
Major Core	18PCY401	Advanced Molecular Spectroscopy	3	1	-	1	4	4
	18PCY402	Analytical Chemistry	3	1	-	1	4	4
	18PCY403	Project Phase-II *(Research & Seminar)*	-	-	16	-	16	8
Major Elective II	18PCY4EA	Bioorganic Chemistry	3	1	-	1	4	4
	18PCY4EB	Materials Chemistry						
	18PCY4EC	Supramolecular Chemistry and Crystal Engineering						
	18PCY4ED	Special Topics in Organic Synthesis						
	18PCY4EE	Nanomaterials and Nanochemistry						
Total			**9**	**3**	**16**	**3**	**28**	**20**

L – Lecture, T – Tutorial, P – Practical, O - Outside Class, C– Credits
Note:* Continuous assessment [Full Internal]

SUMMARY				
Category	**No. of Courses**			
	I Semester	**II Semester**	**III Semester**	**IV Semester**
Core courses	5	5	3	2
Major elective(s)	-	-	1	1
Non-major elective(s)	-	1	1	-
Seminar	-	1	-	-
Project work-Phase I	-	-	1	-
Project work-Phase-II	-	-	-	1
Total number of credits				**82**

Non-Major Electives (offered to other departments)

1. 18PCY2NA Nanochemistry
2. 18PCY2NB Electrochemical Energy Systems
3. 18PCY3NA Chemistry of Biomolecules
4. 18PCY3NB Forensic Science

SYLLABUS

SEMESTER I

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY101	**Chemical Bonding, Molecular Geometry and Group Theory**	**3**	**1**	**-**	**1**	**4**	**4**

Instructional objectives At the end of this course the learner is expected:		**Student Outcomes**				
1.	To understand structure and bonding in molecules	a	b	c		
2.	To understand group theory and its applications in chemistry				d	g

Unit – I The ionic bond

Chemical bond, types of bonds, ionic bond, properties of ionic compounds, factors favouring the formation of ionic compounds, ionization potential, electron affinity and electronegativity, packing of ions in crystals and crystal structures, ccp, hcp, bcc, fcc, radius ratio and structure of ionic lattices, relation between radius ratio and coordination number, stoichiometry and crystal structures.

Lattice energy: definition, Born-Lande equation, factors affecting lattice energy, Born-Haber cycle, enthalpy of formation of ionic compounds and stability, effective nuclear charge, Slater's rule, covalent character in ionic compounds, polarization and Fajan's rules, effects of polarization, solubility, melting points and thermal stability of typical ionic compounds, crystal defects, Schottky defects, F-center and Frenkel defect, non-stoichiometric, interstitial and electron deficient compounds.

Unit – II The covalent bond

Molecular topologies: shared and lone pairs and Lewis structures, isoelectronic and isolobal relationships, hybridization and geometry, VSEPR models, molecular orbital theory, linear combination of atomic orbitals, bonding, antibonding and non-bonding molecular orbitals, MOs of homonuclear diatomic molecules, orbital mixing, heteronuclear diatomic molecules, polar bonds, ionic compounds and molecular orbitals, molecular orbitals of polyatomic molecules.

Unit – III Weak chemical forces and bonding in metals

Vander Waals forces, inclusion compounds, layer, channel and cage structures (gas hydrates and clathrates). Hydrogen bonding: types, non-conventional hydrogen bonding, associated molecules, molecular self assembly, supramolecular architectures formed by weak chemical forces.

Bonding in metals: packing of atoms in metals, band theory of metals and metallic properties, insulators and semiconductors.

Unit – IV Acids and bases

Bronsted-Lowry concept, proton transfer equilibria under aqueous conditions, non-aqueous solvents and acid-base strength, periodic trends in aqua acid strength, oxoacids, anhydrous oxides, Bronsted-Lowry acidity of aqueous cations, Lewis acid- base concept and frontier orbitals, examples of Lewis acids and bases, quantification of Lewis basicity, inductive and steric effects on Lewis acidity and basicity, frustrated Lewis pairs, hard and soft acids and bases, thermodynamic acidity parameters, superacids and superbases.

Unit – V Group theory and its applications

Symmetry elements and operations, point groups, groups and classes of symmetry operations, non-degenerate representations, character table, reduction formula, character of matrices, degenerate representations, applications to molecular vibrations (IR and Raman activity) and chirality.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. D. F.Shriver, P. W.Atkins and C. H. Langford, *Inorganic Chemistry*, 3rdEd., Oxford University Press, London, 2001.
2. K. F.Purcell and J. C.Kotz, *Inorganic Chemistry*, Saunders, Philadelphia, 1976.
3. J. E.Huheey, E. A.Keiter and R. L. Keiter, *Inorganic Chemistry*, 4thEd., Harper and Row, NewYork, 1983.
4. A.Vincent,*Molecular Symmetry and Group Theory. A Programmed Introduction to Chemical Applications*, JohnWiley & Sons Ltd, 1977.
5. F. Albert Cotton, *Chemical Applications of Group Theory*, 2ndEd., John Wiley & Sons, 1971.

Unit-I: Chapter 3 (Shriver), Chapter 3, 4, 6(Huheey).
Unit-II: Chapter 2 (Shriver), Chapter 5(Huheey).
Unit-III: Chapter 7(Huheey), Chapter 3, part 1(Cotton)
Unit – IV: Chapter 4, (Shriver), Chapter 5(Purcell), Chapter 7 and 9(Huheey)
Unit-V: Chapter 2, Part 1 and Chapter 7, Part 2 (Cotton), Chapter 2(Purcell).

References

1. F. A. Cotton, G. Wilkinson, C. A.Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6thEd., Wiley Interscience, New York, 1988.
2. T. Moeller, *Inorganic Chemistry, A Modern Introduction*, John Wiley, New York, 1982.
3. J.D. Lee, *Concise Inorganic Chemistry*, 5th Ed., Blackwell Publishing, Oxford, 2006.
4. A. R. West, *Solid State Chemistry and its Applications*, John Wiley & Sons, New York, 1989
5. L.Smart and E. Moore, *Solid State Chemistry An Introduction*, 2nd Ed., Nelson Thornes Ltd, Cheltenham, 1996.
6. G.L.Miessler, P.J.Fischer and D.A. Tarr, *Inorganic Chemistry*, 5th Ed., Pearson, New York, 2014.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY102	**Classical and Statistical Thermodynamics**	**3**	**1**	**-**	**1**	**4**	**4**

Instructional objectives	**At the end of this course the learner is expected:**	**Student Outcomes**				
1.	To understand the basic principles of classical thermodynamics		**b**	**c**	**d**	
2.	To acquaint the student with the fundamental concepts of statistical and non-equilibrium thermodynamics	**a**	**b**			**g**

Unit- I Classical thermodynamics I

First law of thermodynamics, concept of work and heat, enthalpy and heat capacities, second law of thermodynamics, physical significance of entropy, direction of spontaneous change and dispersal of energy, Carnot cycle, efficiency of heat engine, coefficient of performance of heat engine, Gibbs function, Gibbs–Helmholtz equation, Maxwell relations.

Unit - II Classical thermodynamics II

Thermodynamic equation of state, thermodynamics of systems of variable composition, partial molar quantities, partial molar volume, chemical potential, Gibbs-Duhem equation,experimental determination of fugacity of real gases, third law of thermodynamics, absolute entropies, determination, exceptions to third law, unattainability of absolute zero.

Unit – III Statistical thermodynamics I

Introduction: Macro and micro states, ensembles (microcanonical and canonical), Maxwell-Boltzmann statistics, Boltzmann- Planck equation, Fermi-Dirac and Bose-Einstein statistics, negative absolute temperatures, partition function, evaluation of the partition function translational partition function, rotational partition function, vibrational partition function, electronic partition and nuclear partition function.

Unit – IV Statistical thermodynamics II

Thermodynamic functions in terms of the partition function, internal energy, entropy, Helmholtz function, pressure, Gibbs function, residual entropy, equilibrium constant, isotope effects, molecular interpretation of the basic laws of thermodynamics, average energies and equipartition principle, heat capacity of monoatomic gases, population inversion, negative Kelvin temperature, Einstein's and Debye's theories of heat capacities of solids, nuclear spin statistics, statistical basis of entropy of H_2 gas, ortho and para nuclear states, calculation of entropy in terms of ortho- para ratio, residual entropy of H_2 at 0 K.

Unit – V Non-equilibrium thermodynamics

Introduction, near equilibrium process, general theory, conservation of mass and energy, entropy production in chemical reactions, entropy production and entropy flow in open systems, transformation properties of rates and affinities, Onsager's theory, irreversible thermodynamics and biological systems, oscillatory reactions.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. K. Rajaram and J.C. Kuriacose, *Thermodynamics For Students of Chemistry*, 2nd Ed., S.L.N. Chand and Co, Jalandhar,1986.
2. I.M. Klotz and R.M. Rosenberg, *Chemical thermodynamics*, 6thEd., W.A.Benjamin Publishers, California, 1972.
3. P. W. Atkins,J. De Paula, *Physical Chemistry*, 9thEd., Oxford University Press, Oxford, 2010
4. M.C. Gupta, *Statistical Thermodynamics*, New Age International, Pvt. Ltd, New Delhi, 1995.
5. B. R. Puri, L.R. Sharma and M.S. Pathania, *Principles of Physical Chemistry*, 46th Ed., Vishal Publishing Co., 2014.

   Unit-I: Chapter 2, 3 and 5(Atkins)
   Unit-II: Chapter 6, 7(Atkins)
   Unit-III: Chapter 19, 20 (Atkins)
   Unit-IV: Chapter 19, 20 (Atkins)
   Unit-V: Chapter 36 (Puri)

References

1. D.A. McQuarrie and J.D.Simon, *Physical Chemistry, A Molecular Approach*, Viva Books Pvt. Ltd., New Delhi, 1999.
2. R.P.Rastogi and R.R Misra, *Classical Thermodynamics*, Vikas Publishing, Pvt. Ltd., New Delhi, 1990.
3. S.H. Maron and J.B. Lando, *Fundamentals of Physical chemistry*, MacMillan Publishers, New York, 1974.

Course Nature : Theory
Assessment Method (Max.Marks: 100)

In Semester	Assessment Tool	Cycle Test I	Cycle Test II	Model Examination	Assignment	Attendance	Total
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY103	**Organic Chemistry I - Structure and Reactivity**	**3**	**1**	**-**	**1**	**4**	**4**

Instructional objectives **At the end of this course the learner is expected:**		**Student Outcomes**				
1.	To gain knowledge about basic principles of organic chemistry including stereochemistry	**a**	**b**	**c**		
2.	To acquire knowledge on nucleophilic and electrophilic substitution reactions			**c**	**d**	**g**

Unit – I Principles of structure and reactivity

Review of basic principles of structure and bonding, hybridisation, conjugation, Important properties of organic molecules: dipole moments, inductive effect (+I, -I), mesomeric effect, resonance effect, steric effect, aromaticity and anti-aromaticity, Hückel's rule, y-aromaticity, homo-aromaticity, neutral and charged aromatic systems (3, 4, 5, and 7- membered ring systems), annulenes and fused rings systems, heteroannulenes, aromaticity of heterocycles.

Types of mechanisms, transition states and intermediates,thermodynamic and kinetic requirements, Hammond postulate, Curtin-Hammett principle, methods of determining mechanisms, isotopic effects, generation, structure, stability, and reactivity of carbocations, carbanions, free radicals, carbenes, nitrenes and benzyne, non-classical carbocations, the Hammett equation and linear free energy relationship (sigma-rho) relationship, Taft equation and its application.

Unit – II Stereochemistry

Stereochemistry: conformational analysis of acyclic and cyclic systems, effect of conformation on reactivity, elements of symmetry, chirality, molecules with more than one chiral center, projection formulae (i) Fischer (ii) Sawhorse (iii) Newman (iv) Flying Wedge, threo and erythro isomers, racemic modification, methods of resolution, specific rotation, optical purity and enantiomeric excess, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective reactions, optical activity in the absence of chiral carbon.

Unit – III Nucleophilic additions to carbonyl compounds

Nucleophilic addition to carbonyl compounds, stereochemistry of nucleophilic additions, Cram's rule, Felkin-Anh model,chemistry of imines, enolates, keto-enol tautomerism, condensation reactions of carbonyl compounds, aldol condensations (acid and base catalyzed aldol condensation, crossed aldol condensation, Claisen-Schmidt condensation, directed aldol condensations, Mukaiyama aldol condensation, Claisen ester condensation, Dieckmann reaction, Stobbe condensations, Knoevenagel condensations, 1,4-conjugate additions (Michael addition), Robinson annulation, Wittig reactions, Mannich reactions, nucleophilic addition to isocyanates and isothiocyanates, esterification reactions and ester hydrolysis.

Unit – IV Aliphatic and aromatic nucleophilic substitution

Nucleophilic substitution reactions, SN1, SN2, SNi and neighbouring group mechanisms, nucleophilic substitutions at allylic, aliphatic and vinyl carbons, effect of substrate, nucleophile, leaving group, and medium, stereochemistry of nucleophilic substitution, ambident nucleophiles, aromatic nucleophilic substitutions, SNAr, SN1 and benzyne mechanisms, Sommelet-Hauser, Von Ritcher and Smiles rearrangement, Bucherer and Rosenmund reactions.

Unit – V Aromatic and aliphatic electrophilic substitution

Aromatic electrophilic substitution, mechanism and reactivity, selectivity and orientation, the effect of leaving group, nitration, nitrosation and diazonium coupling, sulphonation, chlorination, bromination, Friedel-Crafts alkylation, acylation and arylation,aliphatic substitution mechanisms, SE2, SEi and SE1, addition-elimination and cyclic mechanisms, halogenations of ketones, aldehydes and carboxylic acids, aliphatic diazonium coupling, sulphonation, sulphenylation, acylation, Stork enamines, carbene and nitrene insertions, Kolbe-Schmidt reaction.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. J.Clayden, N. Greeves, S.Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, 2001.
2. M.B. Smith & J. March, *March's Advanced Organic Chemistry*, 5th Ed., John Wiley & Sons, New York, 2001.
3. F.A. Carey and R.J.Sundberg, *Advanced Organic Chemistry*, Part A and Part B, Kluwer Academic/Plenum Publishers, New York, 2004.

Unit-I: Chapter 9, Part 1 (Smith), Chapter 11 (Carey)
Unit-II: Chapter 4, Part 1 (Smith), Chapter 7 (Carey)
Unit-III: Chapter 15, Part 2 (Smith), Chapter 17 (Carey)
Unit-IV: Chapter 10, 13, Part 2 (Smith), Chapter 8, 20 (Carey)
Unit-V: Chapter 11, 12, Part 2(Smith), Chapter 12(Carey)

References

1. P. Sykes, *A Guide book to Mechanism in Organic Chemistry*, 6th Ed.,Orient Longman Ltd, New Delhi, 1997.
2. S.M. Mukherjee and S.P.Singh, *Reaction Mechanism in Organic Chemistry*, 1stEd., Macmillan India Ltd., New Delhi, 1990.
3. T.H. Lowry and K.S.Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Ed.,Addison- Wesley Longman Inc., 1998.
4. E. L. Eliel, *Stereochemistry of Carbon Compounds*, Tata-McGraw Hill, 2000.
5. P.S. Kalsi, Stereochemistry, 3rdEd., New Age International Publishers, 1995.
6. D. Nasipuri, *Stereochemistry*, Allied Publishers, 2003.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Atten dance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY104	**Main Group Elements and Nuclear Chemistry**	**3**	**1**	**-**	**1**	**4**	**4**

Instructional objectives **At the end of this course the learner is expected:**		**Student Outcomes**				
1.	To gain knowledge about main group chemistry.		**b**		**d**	**g**
2.	To understand the basics of nuclear chemistry.	**a**	**b**	**c**		

Unit – I Main group chemistry-I

Chemical properties of s-block metals: reaction with water, air, nitrogen, uses and their compounds, compounds of *s*-block metals, oxides, hydroxides, peroxides, superoxides, preparation and properties, oxo salts, carbonates, bicarbonates, nitrates, halides and polyhalides, anomalous behavior of Li and Be, complexes of *s*-block metals, complexes with crown ethers and cryptands, biological importance, organometallic compounds of Li, Mg and Be, synthesis, reactivity and bonding.

Unit – II Main group chemistry-II

Polymorphism of carbon, phosphorus and sulfur, catenation and heterocatenation, allotropy of carbon, carbides, salt like carbides, interstitial carbides, covalent carbides, silicates, ortho, pyro, cyclic, chain, sheet, three dimensional silicates and their properties and structures, silicates in technology-alkali silicates, ceramics, glass, organosilicones, preparation, structures, applications.

Synthesis, structure and bonding in polyanions and isopolyanions of phosphorous, vanadium, chromium, molybdenum and tungsten, hetero poly anions of molybdenum and tungsten, oxides and oxyacids of Se and Te, homocyclic inorganic systems $p\pi$-$p\pi$ and $p\pi$-$d\pi$ bonding, structure and properties of interhalogen compounds,[ClF, ICl, ClF_3, BrF_3, IF_3, ClF_5, BrF_5, IF_5] poly halides, psuedohalogens,[cyanide, thiocyanate and azide] and xenon compounds.

Unit – III Main group chemistry-III

Boron oxides and oxoacids, borates and organic compounds containing boron-oxygen bonds, boron sesquioxide, borates, borax, sodium peroxoborates, chemistry of B-N compounds, aminoboranes, borazines, polyborazines, boroxines and boron nitrides, compounds of boron with oxygen, chemistry of P-N compounds, synthesis and reactivity of phosphazene and its polymers, theories of bonding, electronic structure and aromaticity, chemistry of S-N compounds, synthesis and reactivity of S_4N_4,S_2N_2,$S_3N_3Cl_3$and poly thiazyl$(SN)_x$ compounds.

Unit – IV Main group chemistry-IV

Boronhydrides, reaction with ammonia, hydroboration, structure of boranes, borohydrides and their uses, boron and multicentre bonding, boron cages, vacuum technique of synthesis, lower and higher boranes reactions, structure and bonding, topological treatment, Wade's rule, styx numbers, carboranes, metallocarboranes, other hetero atom boron derivatives.

Metal atom cluster, di, tri, tetra, and hexanuclearity metal clusters, cluster structure based on electron counting schemes, capping rule, isoelectronic andisolobal analogy, structure implications, relationship between fragments, isolobal relationships between main-group and transition metal fragments, metal-ligand complexes vs heteronuclear clusters, $d\pi$-$p\pi$ bonding,examples.

Unit – V Nuclear chemistry

Composition of nucleus, nuclear size, nuclear forces, packing fraction, nuclear density, mass defect, binding energy of the nucleus, nuclear models, concept of nuclear spin.

Radioactivity, radioactive disintegration, radioactive decay and half-life, Geiger-Nuttall rule, radioactive equilibrium, steady state, transmutation of elements, group displacement rule, nuclear stability, radioactive series, isotopes, isobars, isotones, separation of isotopes, determination of atomic masses, artificial radioactivity, induced radioactivity, transuranic elements, nuclear coulombic energy barrier, q values of nuclear reactions, nuclear fission, nuclear fusion.

Detectors: scintillation counter, gas ionisation chamber, proportional counter, Cerenkov counter, accelerators, cyclotron, synchrocyclotron, betatron, applications of radioactivity, activation analysis, isotopic dilution technique, radiometric titration.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. D. F. Shriver and P. W. Atkins, *Inorganic Chemistry*, 5thEd.,W. H. Freeman and Co, London, 1999.
2. J. E. Huheey, E. A. Kieter and R. L. Keiter, *Inorganic Chemistry*, 4thEd., Harper Collins, New York, 1993
3. F. A. Cotton, G. Wilkinson, C. Murillo and M. Bochman, *Advanced Inorganic Chemistry*, 6thEd., John Wiley, New York, 1999.
4. N.N.Greenwood and A. Earnshaw, *Chemistry of the Elements,* Pergamon Press, Oxford, 1984.
5. H. J. Arnikar, *Essentials of Nuclear Chemistry*, 4th Ed., New Age International, New Delhi, 1995.

   Unit-I: Chapter 11, 12 (Shriver), Chapter 23, Part 2 (Cotton).
   Unit-II: Chapter 16, 17, 18 (Shriver), Chapter 13, Part 2, (Cotton).
   Unit-III:Chapter 13, 14, 16 (Shriver), Chapter 5, 13, 17, 18,Part 2 (Cotton).
   Unit-IV: Chapter 13, 14 (Shriver), Chapter 5, Part 2 (Cotton).
   Unit-V: (Arnikar).

References

1. J.D. Lee, *Concise Inorganic Chemistry*, 5thEd.,Blackwell Science, London, 1996.
2. R.D. Madan, *Modern Inorganic Chemistry*, S. Chand & Company Ltd, NewDelhi, 2004.
3. B. Douglas and A. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Ed., John Wiley & Sons, Inc, 2001.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY105	Physical Chemistry Laboratory	-	-	6	0	6	3

Instructional objectives At the end of this course the learner is expected:		Student Outcomes				
1.	To motivate the students to understand the principles of chemical kinetics, potentiometric and conductometric titrations.	b	e	f		
2.	To impart knowledge about the phase transformations of different systems.		e		h	k

LIST OF EXPERIMENTS

1. Determination of rate constant of acid hydrolysis of an ester.
2. Determination of molecular weight of substances by Rast method.
3. Determination of critical solution temperature (CST) of phenol- water system and effect of impurity on CST.
4. Study of phase diagram of two components forming a simple eutectic.
5. Distribution of benzoic acid between water and benzene.
6. Adsorption of oxalic acid/acetic acid on charcoal.
7. Determination of Ea of saponification of ester by conductometry method.
8. Determination of equivalent conductance, degree of dissociation, and dissociation constant of weak acids by conductometry.
9. Determination of relative strength of two acids by conductance measurements.
10. Titration of $AgNO_3$vs halide mixture by potentiometry.
11. Redox titrations (MnO_4^- vs I^- / $Cr_2O_7^{2-}$vs Fe^{2+}) by potentiometry.
12. Determination of dissociation constant of weak acids by potentiometry.

Any eight experiments have to be carried out

References

1. J. B.Yadav, *Advanced Practical Physical Chemistry*, 22nd Ed.,GOEL publishing House, Krishna Prakashan Media Ltd, 2005.
2. V.Venkatesan, R. Veeraswamy and A.R. Kulandaivelu, *Basic Principles of Practical Chemistry*, 2nd Ed., Sultan Chand and Sons Publication, New Delhi,1997.
3. B. P. Levitt, *Findlay'sPractical Physical Chemistry*, 9th Ed.,Longman, London, 1985.

Course Nature : Laboratory					
Assessment Method (Max.Marks: 100)					
In Semester	**Assessment Tool**	**Evaluation of Experiments**	**Observation notebook**	**Model exam**	**Total**
	Marks	**30**	**10**	**10**	**50**
End Semester Weightage					**50**
Total					**100%**

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY201	**Quantum Chemistry and Molecular Spectroscopy**	**3**	**1**	**-**	**1**	**4**	**4**

Instructional objectives At the end of this course the learner is expected:		**Student Outcomes**				
1.	To have a good foundation in the physical and mathematical applications of quantum mechanics.	**a**	**b**	**c**		
2.	To understand the basic principles of molecular spectroscopy.			**c**	**d**	**g**

Unit – I Basics of quantum mechanics

de Broglie's concept, experimental verification, Compton effect, Heisenberg's uncertainty principle, derivation of Schrodinger wave equation, requirements for acceptable wave functions, operators, linear operators, estimating the following quantum mechanical operators: position, momentum, kinetic energy, potential energy, total energy, angular momentum, Hermiticity and Hermitian operators, commutator algebra, evaluation of commutators, eigen functions and eigen values, postulates of quantum mechanics.

Unit – II Applications of quantum mechanics-I

Particle in a one dimensional box, quantisation of energy, normalisation of wave function, orthogonality of the particle in a one-dimensional box wave functions, average position and average momentum of a particle in a one-dimensional box, illustration of the uncertainty principle and correspondence principle with reference to the particle in a one-dimensional box, Schrodinger wave equation for a particle in a three dimensional box and the concept of degeneracy of energy levels, Schrodinger wave equation for linear harmonic oscillator, solution by polynomial method, zero point energy and its consequence.

Unit – III Applications of quantum mechanics-II

Solving of Schrodinger wave equation for rigid rotor, energy of rigid rotor, space quantization, Schrodinger wave equation for hydrogen atom, separation of variables in polar spherical coordinates and its solution, principal, azimuthal and magnetic quantum numbers and their magnitude, probability distribution function, radial distribution function and shape of atomic orbitals (s, p & d).

Unit – IV Molecular spectroscopy - I

Time-dependent states and spectroscopy: Absorption and emission of radiation, selection rules, line shapes and widths, Fourier transform spectroscopy.

Rotation and vibration of diatomic molecules: rigid rotor and harmonic oscillator wave functions and energies, selection rules, a review of microwave and IR spectroscopy, diatomic molecule wave functions, symmetry properties and nuclear spin effects.

Raman effect: rotational and vibrational transitions, polarization of Raman lines, vibration of polyatomic molecules, normal coordinates, rule of mutual exclusion.

Unit – V Molecular spectroscopy - II

Electronic spectroscopy: diatomic molecules, Franck-Condon factor, dissociation and pre-dissociation, rotational fine structure, lasers and laser spectroscopy, XPS-PES.

Spin resonance spectroscopy: spin and an applied field, the nature of spinning particles, interaction between spin and magnetic field, Larmor precession, population of energy levels.

Nuclearmagnetic resonance spectroscopy: hydrogen nuclei, chemical shift, coupling constant, coupling between several nuclei.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. R.K.Prasad, *Quantum chemistry*, 4th Ed., New Age International (P) Ltd., Publishers, 2010.
2. D. A. McQuarrie, *Quantum Chemistry*, 2nd Ed., University Science Books, California, 2008.
3. P.W.Atkinsand R. Friedman, *Molecular Quantum Mechanics*, 5th Ed., Oxford University Press, 2011.
4. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Ed., Tata McGraw Hill, New Delhi, 2008.

   Unit-I: Chapter 2, 3 (Prasad), Chapter 1, 3, 4 (McQuarrie), Chapter 1 (Atkins).
   Unit-II: Chapter 4 (Prasad), Chapter 3, 4, 5 (McQuarrie), Chapter 2 (Atkins).
   Unit-III:Chapter 6,7 (Prasad), Chapter 6, 7 (McQuarrie), Chapter 3 (Atkins).
   Unit-IV: Chapter 1, 2 (Banwell).
   Unit-V: Chapter 6, 7, 8 (Banwell).

References

1. L. Piela,*Ideas of Quantum Chemistry*, 1st Ed., Elsevier Amsterdam 2007.
2. A.K.Chandra, *Introductory Quantum Chemistry*, McGraw Hill, 1974.
3. M.W.Hanne, *Quantum Mechanics in Chemistry*, 2ndEd., Benjamin 1969.
4. I. Levine, *Quantum Chemistry*, 2nd Ed., Allyn and Bacon, 1974.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

Course Code	**Course Title**	**L**	**T**	**P**	**O**	**L+T+P**	**C**
18PCY202	**Organic Chemistry II – Structure and Reactivity**	**3**	**1**	**-**	**1**	**4**	**4**

Instructional objectives **At the end of this course the learner is expected:**	**Student Outcomes**

Unit – I Elimination reactions and additions to carbon- carbon multiple bonds

1.	To understand addition and elimination reactions in organic chemistry.	a	c	d	g	
2.	To gain knowledge about useful oxidation and reduction reactions in organic synthesis.	a	b			
3.	To learn about radicals in organic chemistry.		c		d	g

E2, E1, E1cb and E2C mechanisms and stereochemistry, Hoffmann and Satyzeff rules, effect of substrate, base, leaving group and medium, pyrolytic eliminations.

Addition reactions to double and triple bonds, electrophilic, nucleophilic and free radical additions, orientation and reactivity, stereochemistry of addition reactions, addition to cyclopropane rings.

Addition of hydrogen halides (Markovnikov's rule) and bromine,halohydrin formation, hydroboration (anti-Markovnikov's rule), hydrozirconation, iodo and bromolactonization, oxymercuration etc. nucleophilic addition reactions, hydrogenation reactions (hydrogenation of C=C double bonds, triple bonds, and aromatic rings), Chugaev reaction, Hoffmann degradation, Cope elimination, Bamford-Stevens reaction, Sandmeyer reaction, Nazarov cyclization, Koch reaction.

Unit – II Carbon-carbon bond forming reactions

Grignard reagents, cuprates(Gilman reagent)and other conjugate reactions, olefination (Wittig, Horner–Wadsworth–Emmons, Julia, and Peterson) and cyclopropanation reaction, Bayliss Hillman reaction.

Organoboron compounds, synthesis of organoboranes, synthesis of organoboranes, carbonylation and other one-carbon homologation reactions, homologation via α-halo enolates, stereoselectivealkene synthesis, nucleophilicaddition of allylicgroups from boron compounds.

Organosilicon compounds, synthesis of organosilanes, generalfeatures of carbon-carbon bondforming reactions of organosiliconcompounds, addition reactions with aldehydes and ketones, acylation reactions, conjugate addition reactions.

Organotincompounds, synthesis of organostannanes, carbon-carbon bond forming reactions using tin reagents.

Unit – III Oxidation reactions

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

Unit – IV Reduction reactions

(a)Catalytic hydrogenation (Heterogeneous: palladium/platinum/rhodium/nickel etc; Homogeneous: Wilkinson). Noyori asymmetric hydrogenation. (b) Metal based reductions using Li/Na/Ca in liquid ammonia, sodium, magnesium, zinc, (Birch reduction, Pinacol formation, McMurry, acyloin formation, dehalogenation and deoxygenation) (c) Hydride transfer reagents from Group III and Group IV in reductions. (i) $NaBH_4$,triacetoxyborohydride, L-selectride, K-selectride, Luche reduction, $LiAlH_4$, DIBAL-H, and Red-Al,Meerwein-Pondorff-Verley reduction) (ii) Stereo/enantioselective reductions (chiral boranes, Corey-Bakshi-Shibata reduction),Clemmenson and Wolff-Kishner reduction.

Unit – V Radicals in organic chemistry

Reactions involving free radical intermediates, sources of radical intermediates, nucleophilic and electrophilic radicals, mechanisms of radical reactions, solvent and neighbouring group effects, free radical substitutions at aliphatic and aromatic substrates, cyclization of free radical intermediates, additions to C=N double bonds, fragmentation and rearrangement reactions, intramolecular functionalization by radical reactions.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, 1st Ed., Oxford University Press, 2001.
2. M.B. Smith & J. March, *March's Advanced Organic Chemistry*, 6thEd., John Wiley & Sons, New York, 2007.
3. F.A. Carey and R.A. Sundberg, Advanced Organic Chemistry, Part A and Part B, 5thEd., Kluwer Academic/Plenum Publishers, New York, 2004.

Unit-I: Chapter17 (Clayden), Chapter 15, 17 (Smith), Chapter 6, 12 (Carey).
Unit-II: Chapter 9, 20, 22 (Clayden), Chapter 15,16, 18 (Smith), Chapter 7, 9 (Carey).
Unit-III: Chapter 9, 20, 22 (Clayden), Chapter 19 (Smith).
Unit-IV: Chapter 41 (Clayden), Chapter 19 (Smith), Chapter 5 (Carey).
Unit-V: Chapter 37 (Clayden), Chapter 5, 14 (Smith), Chapter 12 (Carey).

References

1. P. Sykes, *A Guide book to Mechanism in Organic Chemistry*, 6th Ed., Orient Longman Ltd., New Delhi, 1997.
2. S. M. Mukherjee and S.P. Singh, *Reaction Mechanism in Organic Chemistry*, 1st Ed., Macmillan India Ltd., New Delhi, 1990.
3. T.H. Lowry and K.S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Ed., Addison – Wesley Longman Inc, 1998.
4. S.H. Pine, *Organic Chemistry*, 5th Ed., McGraw Hill International Edition, 1987.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

Course Code	**Course Title**	**L**	**T**	**P**	**O**	**L+T+P**	**C**
18PCY203	**Advanced Transition Metal Chemistry**	**3**	**1**	**-**	**1**	**4**	**4**

Instructional objectives At the end of this course the learner is expected:		**Student Outcomes**				
1.	To learn about coordination complexes, their properties and reactions.	**a**	**b**	**c**		
2.	To gain knowledge about lanthanides and actinides.	**a**		**c**	**d**	**g**

Unit – I Coordination chemistry-I

Introduction: monodentate, bidentate, and polydentate ligands, coordination sphere, coordination number, nomenclature of mononuclear and dinuclear complexes, chelate effect, Werner's theory and Sidgwick theory, EAN and formation of metal-metal bond in dimers, stability of complexes, determination of stability constants, Jobs method, stepwise stability constant, overall stability constant, factors affecting stability of coordination compounds, charge of central metal ion, size of central metal ion, chelate ring size, steric effects.

Isomerism: linkage, ionization, hydrate, coordination, coordination position isomerism, geometrical (*cis*and *trans*, and *fac* and *mer*) and optical isomerism.

Unit – II Coordination chemistry-II

Valence bond theory: hybridization, geometry, magnetism, drawbacks of VBT.

Crystal field theory: crystal field effects, assumptions of crystal field theory, crystal field splitting in octahedral and tetrahedral geometries, qualitative crystal field splitting diagrams, high-spin and low-spin complexes, CFSP and factors affecting it, computation of CFSE, evidences of crystal field splitting, spectrochemical series, Jahn-Teller theorem, crystal field splitting in tetragonally distorted octahedral geometry and in square planar geometry, covalency in transition metal

complexes, evidences for covalency, intensity of d-d transitions, spin-spin splitting, hyperfine splitting, adjusted crystal field theory.
MO Theory: metal orbitals and LGOs suitable for σ and π bonding in octahedral geometry, construction of qualitative MO energy level diagram for bonding in octahedral geometry.

Unit – III Coordination chemistry-III

Magnetic properties of tetrahedral and octahedral complexes: para, dia, ferromagnetism and antiferro magnetism, determination of magnetic properties, Gouy's method, anomalous magnetic moment, thermal effects, single molecular magnets, spin and orbital contribution quenching, spin cross over rule, microstates of electron configuration in free atoms and ions, term symbols for equivalent and nonequivalent electrons, possible term symbols for given configuration, p^2 - d^2splitting of terms in square planar, tetrahedral, octahedral fields, electronic spectra of various complexes, selection rules, spin orbit coupling, assignment and intensities of transitions, Orgel (d^1 to d^9 octahedral and tetrahedral complexes) and Tanabe Sugano diagrams(d^1,d^6 complexes and its applications), calculation of D0 and b and Racah parameters, examples fromd^2, d^3 d^7, d^8 octahedral complexes, charge transition spectra of metal complexes.

Unit – IV Reaction mechanisms in coordination compounds

Ligand substitution reactions in octahedral, square planar complexes, labile and inert complexes (application of VBT, MOT), dissociation, association mechanism, mechanism of hydrolysis reactions, acid hydrolysis, base hydrolysis, anation reactions, trans effect, trans influence, trans effect and its application, theories of trans effect, thermodynamic and kinetic stability of complexes, factors affecting stability of metal complexes, experimental determination of stability constant of complexes.
Electron transfer reactions, one electron transfer reactions, inner sphere mechanism, outer sphere mechanism, Marcustheory and its applications, two electron transfer reactions, complementary and non - complementary electron transfer reactions, synthesis of coordination compounds using electron transfer reactions, metal assisted reactions, aldol condensation, ester hydrolysis, phosphate ester, aminoesters and amide hydrolysis, template effect, synthesis of macrocyclic ligands, reaction of coordinated ligands.

Unit – V Lanthanides and actinides

Lanthanides: lanthanide series, abundance and natural isotopes, lanthanide contraction, similarity in properties, occurrence, oxidation states, chemical properties of Ln(III)cations, magnetic properties, colour and electronic spectra of lanthanide compounds, separation of lanthanides, solvent extraction, ion exchange, chemical properties of Ln(III) metal ions.

Actinides: actinide series, abundance and natural isotopes, occurrence, preparation of actinides, oxidation states, general properties, the later actinide elements, uranium-occurrence, metallurgy; chemical properties of hydrides, oxides, and halides, complexes of lanthanides and actinides.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. D. F. Shriver and P. W. Atkins, *Inorganic Chemistry*, 3rdEd., W. H. Freeman and Co, London, 1999.
2. J. E. Huheey, E. A. Kieter and R. L. Keiter, *Inorganic Chemistry*, 4thEd., Harper Collins, New York, 1993
3. F. A. Cotton, G. Wilkinson and P.L.Gaus, *Basic Inorganic Chemistry*, 3rdEd., John Wiley, New York, 2008.
4. N.N. Greenwood and A.Earnshaw, *Chemistry of the Elements*, 2nd Ed., Pergamon Press, Oxford, 2005 (Reprint).
5. B.Douglas, D.McDaniel and J.Alexander, Concepts and Models of Inorganic Chemistry, 3rd Ed., Wiley, 2013.

   Unit-I: Chapter 11, 12 (Huheey), Chapter 7 (Shriver), Chapter 6 (Cotton), Chapter 19 (Greenwood), Chapter 9(Douglas)

   Unit-II: Chapter 11, 12 (Huheey), Chapter 20 (Shriver), Chapter 6 (Cotton), Chapter 19 (Greenwood),Chapter 9, 10 (Douglas)

   Unit-III: Chapter 11 (Huheey), Chapter 20 (Shriver), Chapter 6 (Cotton), Chapter 19 (Greenwood), Chapter10 (Douglas)

   Unit-IV: Chapter 13 (Huheey), Chapter 21 (Shriver), Chapter 6 (Cotton), Chapter 19 (Greenwood), Chapter 11 (Douglas)

   Unit-V: Chapter 14 (Huheey), Chapter 23 (Shriver), Chapter 26, 27 (Cotton), Chapter 30, 31 (Greenwood),Chapter 15(Douglas)

References

1. R.D. Madan, *Modern Inorganic Chemistry*, S. Chand & Company Ltd., NewDelhi, 2004.
2. Tobe, M. L.; Burgess, J. *Inorganic Reaction Mechanisms*, Addison Wesley Longman, 1999.
3. R. L. Dutta and A. Syamal, *Elements of Magnetochemistry*, Affiliated East-West PVT Ltd, 1993.
4. O. Kahn, *Molecular Magnetism*, Wiley-VCH Inc., 1993.
5. F. Basoloand Pearson, *Inorganic Reaction Mechanisms*, 2nd ed., Wiley Interscience, 1969.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**

	Marks	10	10	20	5	5	50%
End Semester Weightage							**50%**
Total							**100%**

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY204	**Organic Chemistry Laboratory**	**-**	**-**	**6**	**-**	**6**	**3**

Instructional objectives At the end of this course the learner is expected:		**Student Outcomes**				
1.	To understand the separation methods of organic mixtures.	b	e	f	h	k
2.	To impart knowledge in the synthesis of organic compounds.	b	e		h	

I. Analysis of an organic mixture containing two components.

Pilot separation, bulk separation, analysis, derivatization.

a. Detection of elements (N, Cl, S) by Lassaigne's test

b. Detection of the following functional groups by systematic chemical analysis: aromatic amino (-NH_2), aromatic nitro (-NO_2), amido (-$CONH_2$, including imide), phenolic –OH, carboxylic acid (-COOH), carbonyl (>C=O); only one test for each functional group is to be reported.

Any two mixtures can be given

II. Preparation of Organic compounds (Single stage)

(a) 2,4,6-trinitrophenol(picric acid)from phenol (nitration)
(b) Benzophenoneoxime from benzophenone (addition reaction)
(c) Benzophenoneoxime to benzanilide(rearrangement)
(d) 4-Nitrobenzoic acid to 4-nitrobenzanilide (Substitution)
(e) o-Chlorobenzoic acid from anthranillic acid (Sandmeyer reaction)
(f) p-Benzoquinone from hydroquinone (oxidation)
(g) 2,4,6-Tribromophenol from phenol (bromination)

Two stage synthesis

1. Benzaldehyde → Benzalacetophenone → Epoxide
2. 4-Nitro toluene → 4-Nitro benzoic acid → 4-Amino benzoic acid
3. Resorcinol → 4-methyl-7-hydroxy coumarin → 4-Methyl-7-acetoxy coumarin
4. Cyclohexanone → Phenyl hydrazone → 1,2,3,4-Tetrahydrocarbazole
5. Hydroquinone → Hydroquinone diacetate → 1,2,4-Triacetoxy benzene
6. Acetanilide → p-Acetamidobenzenesulphonyl chloride → p-Acetamidobenzene sulphonamide
7. p-Amino phenol → p-Acetyl amino phenol → p-Ethoxy acetanilide

At least four preparations have to be carried out

III. Spectroscopic Techniques

a)Compounds synthesized by one stage reaction have to be characterized by modern spectroscopic techniques (UV-Vis, FT-IR, NMR).

IV. Gas chromatography

1. Resolution of mixtures-hydrocarbons, alcohols.
2. Determination of Rf values of various organic compounds

References

1. Vogel, *A Textbook of Practical Organic Chemistry*, 5th Ed., Prentice Hall, 1996.
2. Fieser and Fieser, *Reagents in Organic Synthesis*, Wiley, 2006.
3. Mann &Saunders, *Practical Organic Chemistry*, 4thEd., Longmans, 1960.
4. H. T. Clarke., *A Handbook of Quantitative & Qualitative Analysis*, Arnold Heinemann, 1975.

Course Nature : Laboratory					
Assessment Method (Max.Marks: 100)					
In Semester	**Assessment Tool**	**Evaluation of Experiments**	**Observation notebook**	**Model exam**	**Total**
	Marks	**30**	**10**	**10**	**50**
End Semester Weightage					**50**
Total					**100%**

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY205	Inorganic Chemistry Laboratory	-	-	6	-	6	3

Instructional objectives **At the end of this course the learner is expected:**		**Student Outcomes**				
1.	To enable students to understand the principles behind semi-micro qualitative analysis.	b		f	h	k
2.	To learn about electroanalytical and photometry techniques.		e	f		k

I. Semi – micro qualitative analysis:

Analysis of mixtures containing two familiar and two less familiar cations from the following W, Pb, Se, Te, Mo, Cu, Cd, As, Sb, Ce, Be, Th, Zr, Ti, V, Cr, Mn, U, Ni, Co, Zn, Ca, Ba, Sr, Li (insoluble and interfering anions may be avoided).

Any three combinations of different salts.

II. Synthesis of metal complexes

1. Potassium tris(oxalato)ferrate(III),
2. Hexaamminecobalt(III) chloride,
3. Tris(thiourea)copper(I) sulphate.

Any two of the above can be selected.

III. SPECTROPHOTOMETRY

1. Determination of Iron/Cobalt.
2. Determination of dissociation constant of an acid - base indicator.

3. Determination of Chromium.
4. Determination of Manganese in steel
5. Determination of an organic dye and dye degradation

Any two of the above can be selected.

IV. FLAME PHOTOMETRY

1. Determination of sodium, potassium and calcium
2. Determination of potassium in combined fertilizer
3. Determination of calcium in wine
4. Simultaneous determination of sodium and potassium in soil samples
5. Determination of Arsenic in water samples

Any two of the above can be selected.

References

1. Vogel, Revised by G Svehla, *Qualitative Inorganic Analysis*, 6th Ed., Longman, 1987.
2. V.V. Ramanujam, *InorganicSemi-micro Qualitative Analysis*, The National Publishing Co, Chennai, 1974.
3. Willard, Merit, Dean and Settle, *Instrumental Methods of Analysis*, 6th Ed, CBS Publ. & Distributors, 1986.
4. I. Vogel, *Text Book of Quantitative Analysis*, 4th Ed., ELBS, 1978.
5. Gray D. Christian & James, E. O'Relly, Allyn& Bacon Inc, *Instrumental Analysis*, 2nd Ed., 1986.
6. D.A.Skoog and West, *Principles of Instrumental Analysis*, 6th Ed., Saunders College Pub. Co.,2006.

Course Nature : Laboratory					
Assessment Method (Max.Marks: 100)					
In Semester	**Assessment Tool**	**Evaluation of Experiments**	**Observation notebook**	**Model exam**	**Total**
	Marks	**30**	**10**	**10**	**50**
End Semester Weightage					**50**
Total					**100%**

SEMESTER III

Course Code	**Course Title**	**L**	**T**	**P**	**O**	**L+T+P**	**C**
18PCY301	**Organometallic and Bioinorganic Chemistry**	**3**	**1**	**-**	**1**	**4**	**4**

Instructional objectives	**At the end of this course the learner is expected:**	**Student Outcomes**				
1.	To understand the basics of organometallic chemistry.	**a**		**c**		
2.	To gain knowledge about bioinorganic molecules and their role in biology		**b**		**d**	**g**

Unit – I Introduction to organometallic chemistry

Type of ligands and eighteen electron rule, transition metal carbonyl complexes, substitutes for carbonyl ligands, non-carbon ancillary ligands, ligand substitution reactions, ligand insertion reactions, carbene complexes, transition metal organometallics: square planar complexes, metal alkyls, metal alkylidenes, metal alkylidynes and metal arenes, Vaskas complex, isolobal analogy, fluxional properties of organometallics.

Unit – II π Complexes of unsaturated molecules, reactions and properties

Synthesis, structure, bonding and reactivity of transitional metal complexes with alkenes, cyclopentadienyl, cycloheptatriene, cyclooctatetraene, benzenoid, π-allyl, and enyl systems, metathesis reactions, migratory insertion reaction with alkynes, C – C single bond formation reactions, oxidative addition, transmetallation, reductive elimination, insertion, and (β-hydride and alkyl) elimination reactions,reactions involving organocopper and palladium intermediates and other transition metals, Suzuki, Stille, Negishi and Ullman coupling reactions with mechanism, Heck reaction with mechanism.

Unit – III Catalytic and stoichiometric reactions and their applications

Homogeneous catalysis: hydrogenation, hydroformylation, acetic acid synthesis, heterogeneous catalysis: Fischer-Tropsch reaction and Ziegler-Natta polymerization, olefin oxidation, isomerisation, addition of HX to olefins, carbonyl insertion, hydride elimination, abstraction, cyclooligomerisation, ethylene dimerization using $RhCl_3$ as catalyst,asymmetric catalysis, organometallic compounds in medicine, agriculture, horticulture, and other industries.

Unit – IV Bioinorganic moleculesand their function

Photosystems, porphyrins, ion (Na^+ and K^+) transport, oxygen binding, transport and utilization, electron transfer reactions, nitrogen fixation, metalloenzymes containing magnesium, molybdenum, iron, cobalt, copper and zinc, role of metal complexes in medicine.

Unit – V Role of biologically active moleculesand their characterization

Oxygen binding properties of heme (haemoglobin and myoglobin) and non-heme proteins hemocyanin & hemerythrin), their coordination geometry, electronic structure and co-operativity effect, electron transfer proteins, active site structure and functions of ferredoxin, rubridoxin and cytochromes and their comparisons,characterization techniques: UV-Vis, Raman, X-Ray crystallography, paramagnetic NMR and EPR spectroscopy, EXAFS, magnetic susceptibility and electrochemistry.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. B. D. Gupta and A. J. Elias, *Basic Organometallic Chemistry: Concepts, Syntheses and Application,* UniversitiesPress, 2013.
2. R. C.Mehrotra, and A. Singh, *OrganometallicChemistry: A Unified Approach*, Wiley Eastern, 2000.
3. S. Lippard and J. Berg, *Principles of Bioinorganic Chemistry*, Univ. Science Books, 1994.

Unit-I: (Gupta) (Mehrotra).
Unit-II: (Gupta) (Mehrotra).
Unit-III:(Gupta) (Mehrotra).
Unit-IV: (Lippard and Berg).
Unit-V: (Lippard and Berg).

References

1. G. O. Spessard and G. L. Miessler, *Organometallic Chemistry*, Prentice Hall, Upper Saddle River, NJ, 1997.
2. C. Elschenbroich, *Organometallics: A Concise Introduction* Wiley-VCH: Weinheim, 2006.
3. D. Steinborn, *Fundamentals of Organometallic Catalysis* Wiley-VCH, 2012.
4. I. Bertini, H. B. Gray, S. J. Lippard, and J.S. Valentine, *Bioinorganic chemistry,* University Science Books, 1994.
5. E.I.Stiefel, and G. N. George, *Ferredoxins, hydrogenases, and nitrogenases: Metal-sulfide proteins. Bioinorganic Chemistry,* 1994.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

Course Code	**Course Title**	**L**	**T**	**P**	**O**	**L+T+P**	**C**
18PCY302	**Chemical Kinetics and Surface Chemistry**	**3**	**1**	**-**	**1**	**4**	**4**

Instructional objectives At the end of this course the learner is expected:		Student Outcomes				
1.	To help the student understand the basic principles of chemical kinetics.	a	b	c		
2.	To appreciate the area of surface chemistry and its role in catalysis and electrochemistry.	a		c	d	g

Unit – I Theories of reaction rates

Simple collision theory, absolute reaction rate theory (ARRT), thermodynamic treatment, potential energy surfaces, application of ARRT to simple bimolecular process, chain reactions, general characteristics, study of kinetics of chain reaction like H_2-Br_2 reaction, decomposition of acetaldehyde and N_2O_5,study of H_2- O_2explosive reactions, theory of unimolecular reactions, Lindemann, Hinshelwood, RRKM and Slater treatment, steady state approximation, principle of microscopic reversibility and detailed balancing, kinetic isotope effect.

Unit – II Reactions in solutions

Solvent effects on reaction rates, cage effect, factors determining the reaction rates in solution (based on transition state theory),reactions between ions, ion-dipole and dipole - dipole reactions, structure, significance of volume and entropy of activation, pressure effect, primary and secondary salt effects.

Unit – III Kinetics of complex processes

Kinetics of photophysical and photochemical processes, complex photochemical processes, homogeneous catalysis : general catalytic mechanisms, acid-base catalysis, catalysis by enzymes, influence of concentration (single substrate, double substrate), inhibition, transient, phase kinetics, sigmoid kinetics, kinetics of bacterial growth.

Unit – IV Isotope effects and fast reactions

Equilibrium isotope effects, primary kinetic isotope effects, secondary kinetic isotope effects.
Fast reactions: relaxation kinetics, basic principles of chemical relaxation methods, chemical relaxation in two step and multi step synthesis, experimental methods for the study of relaxation kinetics and applications, temperature jump method, electrical field jump method, ultrasonic relaxation methods, NMR method, diffusion controlled reactions, fluorescence quenching, electrochemical methods, common ion inhibition, flash photolysis.

Unit – V Surface chemistry

Adsorption of gases and vapors on solids, the Langmuir adsorption isotherm, kinetic and statistical derivation of Langmuir adsorption isotherm, adsorption entropies, lateral interactions, the BET and related isotherms, derivation of the BET equation, properties of the BET equation, Langmuir Blodgett films, structure and characterization, mixed LB films, studies of the LB deposition process, thermodynamics of adsorption chemisorption and catalysis, chemisorption, the molecular view, chemisorption isotherms, kinetics of chemisorption, the chemisorption bond.

Electrical aspects of surface chemistry, electrical double layer, Stern treatment of the electrical double layer, free energy of a diffuse double layer, repulsion between two plane double layers, zeta potential, electrophoresis, electro osmosis, streaming potential sedimentation potential electro capillarity, thermodynamics of electro capillary effects.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. K. J. Laidler, *Chemical Kinetics*, 3rdEd., Harper & Row, 1987.
2. K. A. Connors, *Chemical Kinetics - The study of reaction rates in solution*, Wiley - VCH, 1990.
3. C. Kalidas, *Chemical Kinetic Methods*, New Age International Publishers, New Delhi, 1996.
4. P. Atkins and J. de Paula, *Physical Chemistry*, 7thEd., Oxford University Press, Oxford, 2002.
5. A.W. Adamson and A. P. Gast, *Physical Chemistry of Surfaces*, 6th Ed., John Wiley & sons 1997.

Unit-I: (Laidler), (Connors), (Kalidas), (Atkins).
Unit-II: (Laidler), (Connors), (Kalidas), (Atkins).
Unit-III: (Laidler), (Connors), (Kalidas), (Atkins).
Unit-IV: (Laidler), (Connors), (Kalidas), (Atkins).
Unit-V: (Atkins), (Adamson).

References

1. G. D. Billing and K.V. Mikkalsen, *Introduction to molecular dynamics and chemical kinetics*, John Wiley and Sons, 1996.
2. K. J. Laidler, *Physical chemistry with biological application,* Benjamin Cummings Publications Co.,Inc,1980.
3. H. Strehlow and W. Knoche, *Fundamentals of Chemical relaxation,* Verlag Chemie, Weinheim, 1977.
4. C.D.Ritchie, *Physical organic chemistry, The fundamental concepts*, Marcel Dekker, Inc., 1990.
5. P.C. Hiemenz, *Principles of colloids and surface chemistry*,2ndEd.,Marcel DekkerInc., 1986.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY303	**Advanced Organic Chemistry**	**3**	**1**	**-**	**1**	**4**	**4**

Instructional objectives	**Student Outcomes**

At the end of this course the learner is expected:						
1.	To learn about pericyclic reactions and molecular rearrangements.	**a**	**b**		**d**	**g**
2.	To gain knowledge of the basic principles of photochemistry.	**a**		**c**		

Unit - I Pericyclic reactions I

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3 butadiene, 1,3,5- hexatriene, allyl system, classification of pericyclic reactions, FMO approach, Woodward- Hoffman correlation diagram method and perturbation of molecular (PMO) approach for the explanation of pericyclic reactions under thermal and photochemical conditions, electrocyclic reactions: conrotatory and disrotatory motions (4n) and (4n+2), allyl systems and secondary effects.

Unit – II Pericyclic reactions II

Cycloadditions: antarafacial and suprafacial additions, notation of cycloadditions, (4n) and (4n+2) systems with a greater emphasis on (2+2) and (4+4), cycloadditions, (2+2), additions of ketones secondary effects of substitutes on the rates of cycloadditions and chelotropic reactions, FMO approach and perturbation of molecular (PMO) approach for the explanation of sigmatropic rearrangements under thermal and photochemical conditions, suprafacial and antarafacial shifts of hydrogen, sigmatropic shift involving carbon moieties, retention and inversion of configuration, (3,3) and (5,5) sigmatropic rearrangements, Claisen and Cope rearrangements, fluxional tautomerism, aza-Cope rearrangements.

Unit – III Molecular rearrangements

Wagner-Meerwein, pinacol and benzilic acid rearrangements in acyclic and cyclic organic molecules (substituted cyclohexane and decalin), migrating aptitude and their stereochemical outcome, rearrangement involving diazomethane (Wolff and Demjanov rearrangement), Stevens, Sommelet and Wittig rearrangements, Favorskii rearrangement in acyclic and cyclic α-halo ketones, Fries Rearrangement, McLafferty rearrangement, Hoffman, Curtius, Schmidt and Lossen rearrangements and its key reaction intermediates, Beckmann rearrangement and its stereochemistry, Baeyer–Villiger rearrangement in cyclic and acyclic ketones and migratory aptitude of alkyl and aryl groups, Dakin reaction in conversion of benzaldehyde to phenol and salicylaldehyde to catechol.

Unit – IV Retrosynthetic analysis and protecting groups in organic synthesis

Concepts in organic synthesis: retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity, protecting functional groups, protection of NH and OH groups, acetals as protecting groups for diols, protection of carbonyl groups in aldehydes and ketones, protection of the carboxyl group, protection of double and triple bonds.

Unit – V Basic principles of photochemistry

Absorption of light by organic molecules, Jablonski diagram, properties of excited states, mechanism of excited state processes and methods of preparative photochemistry, photochemistry of alkenes and related compounds: isomerization, Di-π-methane rearrangement and cycloadditions, photochemistry of aromatic compounds: ring isomerization and cyclization reactions, photochemistry of carbonyl compounds: Norrish type-I cleavage of acyclic, cyclic, and unsaturated carbonyl compounds, Norrish type-II cleavage, hydrogen abstraction: intramolecular and intermolecular hydrogen abstraction, photoenolization, photocyclo-addition of ketones with unsaturated compounds: Paterno-Buchi reaction, Barton reaction, photodimerisation of α, β-unsaturated ketones, rearrangement of enones and dienones, photo-Fries rearrangement.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. J. Clayden, N.Greeves, S. Warren and P. Wothers, *Organic Chemistry*, 1st Ed., Oxford University Press, 2001.
2. M.B. Smith & J.March, *March's Advanced Organic Chemistry*, 5th Ed., John Wiley & Sons, New York, 2001.
3. F.A. Carey and R.A. Sundberg, Advanced Organic Chemistry, Part A and Part B, 5th Ed., Kluwer Academic/Plenum Publishers, New York, 2004
4. P. G. M. Wuts, *Greene's Protective Groups in Organic Synthesis*, 5th Ed., Wiley, 2014.

References

1. Peter Sykes, *A Guide book to Mechanism in Organic Chemistry*, 6th Ed., OrientLongman Ltd., New Delhi, 1997.
2. S. M. Mukherjee and S.P. Singh, *Reaction Mechanism in Organic Chemistry*, 1st Ed., Macmillan India Ltd., New Delhi, 1990.
3. T.H. Lowry and K.S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rdEd., Addison–Wesley
Longman Inc., 1998.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

MAJOR ELECTIVES I

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY3EA	Advanced Electrochemistry	3	1	-	1	4	4

Instructional objectives At the end of this course the learner is expected:		Student Outcomes				
1.	To understand the theories and concepts of electrochemistry.	a	b			
2.	To gain knowledge about modern areas of electrochemistry like electrocatalysis, photoelectrocatalysis, and bioelectrodics.			c	d	g

Unit – I Ions in solution and electrical double layer

Ions in solution: deviation from ideal behaviour, ionic activity, ion-solvent and ion-ion interactions, expression forfree energy, Debye-Huckel-Bjerrum model, mean activity coefficient, applications of Debye-Huckel limiting law, extent of dissociation of a weak electrolyte in the presence of an inert electrolyte, Debye-Huckel theory of strong electrolytes, transport of ions in solution: electrolytic conduction, Debye-Huckel-Onsager treatment of the conductance of strong electrolyte and its limitations, the electrical double layer, structure of electrical double layer, Helmholtz-Perrin, Guoy-Chapmann and Stern models of electrical double layer, applications and limitations.

Unit – II Electrodics

Basics of electrodics, rates of simple electrode reactions, elementary electron electrode process, Butler-Volmer equation, exchange current density and symmetry factor, experimental determinations, electrode rectification, Nernst equation as a special case of the Butler -Volmer equation, reaction resistance, polarisable & non-polarisable electrodes, low and high field approximations, Tafel equations.

Examples of multi electron reactions, Butler-Volmer equation for a multi step reaction, the concept of rate determining step of an electrode reaction, transfer coefficients and stoichiometric number, electro-chemical reaction mechanisms, electrochemical reaction order, determining the stepwise mechanism of an electrodic reaction, current potential laws for electrochemical systems.

Unit – III Concentration polarization

Types of over voltages, chemical and electrochemical over potentials, phase, activation and concentration overpotentials, diffusion, migration and hydrodynamic modes of transports, the role ofsupporting electrolyte, theory of diffusion over potential, polarography, limiting current density and its importance.

Unit – IV Electrodic reactions of interest

Standard electrodes and electrodes at equilibrium, Ohmic and non-Ohmic behaviors, reactions at an electrode,three electrode system,sign conventions,rates of electrochemical reactions, over potential, chemical & electrochemical conditions for the discharge of ions, electrocatalysis, electrogrowth of metals, hydrogen evolution reactions, electronation of oxygen.

Technological aspects of electrochemistry: corrosion and stability of metals, electrochemical energy conversion, electricity storage.

Unit – V Advanced topics in electrochemistry

Photoelectrochemistry: introduction, band bending at the semiconductor/solution interface, photoexcitation of electrons by absorption of light, surface effects in photoelectrochemistry, photoelectrocatalysis, the photoelectrochemical splitting of water, the photoelectrochemical reduction of CO_2.

Bioelectrochemistry : bioelectrodics, membrane potentials, electrochemical communication in biological organisms, enzymes as electrodes, electron transfer in p450 enzymes, electrochemical sensors, electrochemical biosensors, gas sensors, solid state devices and sensor arrays.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. J.O.M. Bockris and A.K.N. Reddy, *Modern Electrochemistry*, Volumes 1 & 2, Plenum Press, New York. 1988.
2. S.Glasstone, *Electrochemistry*, Affiliated East-West Press, Pvt., Ltd., New Delhi, 1974.
3. A.J.Bard and L.R. Faulkner, *Electrochemical methods –Fundamentals and Applications*,,2nd Ed., John Wiley and Sons, 2001.
4. C.Hamann, A. Hamnett and W. Vielstich, *Electrochemistry*, Wiley, 2007

References

1. D.A.McQuarrie and J.D.Simon, *Physical Chemistry-A Molecular Approach*, Viva Books Pvt. Ltd., New Delhi, 1999.
2. J.Rajaram and J.C. Kuriakose, *Kinetics and Mechanism of Electrochemical Transformations*, Macmillan India Ltd., New Delhi, 1993.
3. R.J Gale, *Spectroelectrochemistry*, Wiley 2010.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY3EB	**Heterocyclic Chemistry and Total Synthesis of Natural Products**	**3**	**1**	**-**	**1**	**4**	**4**

Instructional objectives **At the end of this course the learner is expected:**	**Student Outcomes**

1.	To learn about heterocycles, their structure, properties and synthesis.	**a**	**b**	**c**		
2.	To gain exposure to the field of total synthesis of natural products.				**d**	**g**

Unit – I Introduction

Nomenclature of heterocycles, monocyclic, fused and bridged heterocycles, effect of heteroatoms on organic reactions, comparison with carbogenic compounds, heterocycles in organic synthesis and biomolecules, oxidation and reductions in heterocyclic chemistry.

Unit – II Structural aspects of aromatic and non-aromatic heterocycles

Aromatic heterocycles: classification, criteria of aromaticity, bond lengths, ring current and chemical shifts in ^{1}H NMR-spectra, resonance energy, delocalization energy and Dewar resonance energy, tautomerism in aromatic heterocycles, general trends in the reactivity of aromatic heterocycles.

Strain, bond angle and torsional strain and their consequences in small ring heterocycles, conformation of six-membered heterocycles, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interactions, stereo-electronic effects, anomeric and related effects, hydrogen bonding and intermolecular nucleophilic, electrophilic interactions.

Unit – III Synthesis and reactions of heterocycles

Basic principles of heterocycle synthesis, cyclization and cycloaddition reactions, three-membered and four-memberedheterocycles, synthesis and reactions of azirines,aziridines, pyrrole, thiophene, furan, pyrazole, imidazole, oxazole, thiazole, pyrimidine, pyrazine, benzofurans, indole, benzothiophenes pyridine, quinoline, isoquinoline, six membered rings containing two heteroatoms.

Unit – IV Total synthesis of natural products-I

Total synthesis of the following:
Antibiotics: Penicillin
Alkaloids: Morphine
Terpenes: Forskolin

Unit – V Total synthesis of natural products-II

Woodward's synthesis of reserpine and cholesterol, Corey's synthesis of prostaglandins (E_2, $F_{2\alpha}$), Nicolaou's synthesis of taxol, Danishefsky's synthesis of indolizomycin, Takasago synthesis of menthol.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. T.L.Gilchrist, *Heterocyclic Chemistry*, 3rd Ed.,Prentice Hall,1997.
2. A.R.Katritzky, and C.W.Rees, *Comprehensive Heterocyclic Chemistry*, Pergamon Press,1996.
3. R.R.Gupta, M.Kumar, and V.Gupta,, *Heterocyclic Chemistry,* Vo1.1-3, Springer Verlag,2008.
4. D.T.Davies, *Aromatic Heterocyclic Chemistry*, Oxford Chemistry Primers,1992.
5. K. C.Nicolaou, *Classics in total synthesis*, Wiley, 1996.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	Assessment Tool	Cycle Test I	Cycle Test II	Model Examination	Assignment	Attendance	Total
	Marks	10	10	20	5	5	50%
End Semester Weightage							50%
Total							100%

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY3EC	Polymer Science	3	1	-	1	4	4

Instructional objectives At the end of this course the learner is expected:		Student Outcomes				
1.	To understand the fundamental principles in polymer science.	a	b	c	d	g
2.	To learn about polymer properties and applications.				d	g

Unit – I Introduction to polymers

Basic concepts, monomers, repeat units, degree of polymerization, nomenclature of polymers, linear, branched and network polymers, concept of molecular mass, polydispersity, number average and weight average, viscosity average molecular weight and their statistical equations, molecular weight distribution in linear polymers (step growth and chain polymers).

Unit – II Measurement of molecular weight and techniques of polymerization

Measurement of molecular weights, end group, viscosity, light scattering, osmotic and ultracentrifugation methods, methods of polymerization, bulk polymerization, solution polymerization, emulsion polymerization, suspension polymerization, interfacial polymerization, melt polycondensation, solution polycondensation.

Unit – III Step-growth and chain growth polymerization

Basics of step growth and chain growth polymerization, radical, cationic, anionic and condensation polymerization, copolymerization, reactivity ratios, thermodynamic aspects of polymerization, mechanism of living radical polymerizations: nitroxide mediated polymerization (NMP), metal-catalyzed living radical polymerization, Reversible Addition-Fragmentation chain Transfer (RAFT) radical polymerization, coordination polymerization, ring opening polymerization, click chemistry.

Unit – IV Polymer structure and properties

Types of stereo isomerism in polymers, properties of stereo regular polymers, Flory-Huggins theory of polymer solutions, nature, size and shape of macromolecules in solution, morphology and order in crystalline polymers, configurations of polymer chains, crystalline melting point T_m – melting points of homogenous series, effect of chain flexibility and other steric factors, entropy and heat of fusion, the glass transition temperatureT_g, relationship between T_m and T_g, Relation between T_g and other parameters, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross-linking, DSC, DTA and TGA for polymer characterization, rheological properties.

Unit – V Specialty polymers and polymer processing

Polymer processing: elastomers and fibres, compounding, processing techniques: calendering, die-casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermo forming, foaming, reinforcing and fibre spinning, liquid crystalline polymers, conducting polymers, electroluminescent polymers, inorganic polymers, nanocomposites of polymers, biomedical polymers, properties of commercial polymers: polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. F.W.Billmeyer, *Text Book of Polymer Science*, 3rd Ed., John Wiley & Sons, New York, 2003.
2. V.R.Gowariker, N.V.Viswanathan and J. Sreedhar, *Polymer Science*, New Age International, New Delhi, 2003.
3. H.R.Alcock and F.W.Lamber, *Contemporary Polymer Chemistry*, Prentice Hall,1981.
4. P.J.Flory, *Principles of Polymer Chemistry*, Cornell University press, New York, 1953.
5. G.Odian, *Principles of Polymerization*, 4nd Ed., John Wiley & Sons, New York, 2004.
6. P. Bahadur and N.V. Sastry, *Principles of Polymer Science*, 2nd Ed., Narosa Publishing House, 2005.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

SEMESTER IV

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY401	Advanced Molecular Spectroscopy	3	1	-	1	4	4

Instructional objectives At the end of this course the learner is expected:		Student Outcomes				
1.	To learn the basic principles of molecular spectroscopy and its applications in structure determination.	a		c	d	g
2.	To understand the concept of structural determination of organic compounds.	a	b		d	g

Unit – I UV-visible spectroscopy

Relating electromagnetic spectrum with electronic, vibrational, rotational energy levels of organic molecules, selection rules for electronic transition, Franck-Condon principle, Jablonski diagram and photophysical processes.

Ultraviolet–visible (UV-Vis) spectroscopy: Introduction of electronic excitation, instrumentation, presentation of spectrum, chromism, chromophore, fluorophore etc, studies of conjugated and extended conjugated systems, aromatic systems etc, solvent effects, Woodward rules, Beer-Lambert law, study of photochromic compounds.

Fluorescence spectroscopy: Instrumentation, emission of photochromic compounds, determination of kinetic parameters of short lived photoswitches, fluorescence energy transfer.

Unit – II Infrared (IR) spectroscopy

Major modes of vibration, instrumentation (FT spectrometer), correlation charts and tables, identification of functional groups and hydrogen bonding.

Elemental Analysis & Mass Spectrometry: Qualitative and quantitative elemental analysis, molecular mass determination, determination of molecular formula of an unknown organic substrate, fragmentation and rearrangements.

Unit – III Nuclear magnetic resonance (NMR) spectroscopy

Basic concepts and principles, nuclear spin states, nuclear magnetic moments, mechanism of resonance, chemical shifts, diamagnetic shielding, magnetic anisotropy, spin-spin splitting, coupling constant, first order and second order spectra, CW and FT instrument, ^{1}H and ^{13}C NMR absorption of different types of organic compounds, peak broadening due to exchange process, chemicals shift reagents, chiral resolving agents, study of certain reaction kinetics via NMR spectroscopy, introduction to 2D-NMR: COSY, NOESY, DEPT,INPET, APT, INADEQUATE, basic introduction to solid state NMR.

Unit – IV ESR and Mossbauer spectroscopy

Basic principles and applications of ESR spectroscopy to free radicals, molecules and transition metal complexes, basic principles of Mossbauer spectroscopy, applications on the basis of isomer shifts, electric quadrupole interactions, structural elucidation of $I_2Br_2Cl_4$, I_2Cl_6, Fe^{+2} and Fe^{+3} complexes and Sn^{+2} and Sn^{+4} compounds. Applications of NMR to metal nuclei (examplePt 195 and Sn 119).

Unit – V Structural elucidation of organic compounds

By joint application of UV, IR, NMR and mass spectrometry for simple organic compounds.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. R. M. Silverstein, G. C. Bassler and T. C. Morril, *Spectroscopic Identification of Organic Compounds*,3rd Ed., John Wiley & Sons Inc., 1974.
2. W. Kemp,*Organic Spectroscopy*, Palgrave Macmillan, 1991.
3. C.N.Banwell and E.M. McCash, *Fundamentals of Molecular spectroscopy*, 4thEd., McGraw-Hill, 1972.
4. M-M. Cid, J. Bravo,*StructureElucidation in Organic Chemistry: The search for the right tools*, Wiley-VCH, 2015.
5. N. E. Jacobsen,*NMR Data Interpretation Explained: Understanding 1D and 2D NMR Spectra of Organic Compounds and Natural Products*, Wiley, 2016.
6. D. L. Pavia, G.M. Lampman, G.S. Kriz and J.R. Vyvyan, *Spectroscopy*, India Edition, 2007.
7. J. Mohan, *Organic Spectroscopy: Principles and Applications*, 2nd Ed., Narosa Publishing House, 2007.
8. H.S. Randhawa, *Modern Molecular Spectroscopy*, Macmillan India Ltd., 2003.
9. P. S. Sindhu, *Fundamentals of Molecular Spectroscopy*, 1st Ed., New Age International Publishers, 2006.
10. S. Chandra, *Molecular Spectroscopy*, Narosa Publishing House, 2009.

Unit-I: (Silverstein) (Kemp) (Pavia) (Mohan)
Unit-II: (Kemp) (Pavia) (Mohan)
Unit-III:(Silverstein) (Pavia) (Mohan)
Unit-IV: (Banwell) (Randhawa) (Sindhu) (Chandra)
Unit-V:(Jacobsen) (M-M Cid) (Pavia)

References

1. R. J. Abraham, J. Fisher and P. Loftus, *Introduction to NMR spectroscopy*, 1stEd.,Wiley, 1992.
2. J. R. Dyer, *Application of Spectroscopy of Organic Compounds*, Prentice-Hall, Englewood Cliffs, N.J., 1965.
3. P. S. Kalsi, *Spectroscopy of Organic Compounds*,New Age International, 2007.
4. M. L. Martin, J. J. Delpench and G. J. Martin, *Practical NMR Spectroscopy*,Heyden, London 1980.

5. D. H. William, I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 6th Ed., Tata McGraw Hill Education, 2011.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	Assessment Tool	Cycle Test I	Cycle Test II	Model Examination	Assignment	Attendance	Total
	Marks	10	10	20	5	5	50%
End Semester Weightage							50%
Total							100%

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY402	Analytical Chemistry	3	1	-	1	4	4

Instructional objectives At the end of this course the learner is expected:		Student Outcomes				
1.	To understand the fundamental principles of analytical chemistry.	a	b	c	d	g
2.	To be aware about modern analytical techniques and their uses.			c	d	g

Unit – I Data analysis and good lab practice

Principle of GLP and handling of first aid and safety, storage and handling of chemicals, antidotes, threshold vapour concentration, accuracy, precision, sensitivity, specificity, standard deviation, classification of errors and their minimization, significant figures, criteria for rejection of data, Q-test, T test and F-test, control chart, sampling methods, sampling error, statistical data treatment, standard reference materials.

Unit – II Classical analytical methods

Principle of volumetric analysis, concept of solubility product, common ion effect and their applications in qualitative and volumetric analyses, principles of gravimetric analysis, theories of precipitation, precipitation from homogenous medium, co-precipitation and post precipitation reactions, theories of acid-base, redox, complexometric, and iodimetric titrations, buffer solutions, theories of indicators, acid-base indicators, choice of indicators, redox-metal ion and adsorption indicators, metal ion indicators and their characteristics, limitations of volumetric analysis.

Unit – III Analytical separation and purification techniques

Precipitation, distillation, solvent extraction and separation processes, partition chromatography, column chromatography, thinlayer chromatography (TLC), paper chromatography and their applications.

Ion exchange chromatography: principle, instrumentation with special reference to separation and suppressor columns and applications.
Principles, instrumentation and applications of GC, LC, and HPLC, signal to noise ratio, sources of noise in instrumental analysis.

Unit – IV Electrochemical analysis

Specific and molar conductances, Kohlrausch's law, measurement of dissociation constant, coulometric and conductometric titrations.

Galvanic cells: Introduction to electrochemical cells, standard electrode potential, electrochemical series, Nernst equation.

Potentiometry, ion-selective electrodes, liquid membrane electrodes, polarography and voltammetry principles, voltammograms, equation of voltamogram, modified voltametric methods, cyclic voltammetry, amperometry, anodic stripping voltammetry. Electrochemical sensors, modified electrodes and their applications, electronic tongue, principle, instrumentation, operation and applications.

Unit – V: Thermal analysis

Thermoanalytical methods: principles of thermogravimetric analysis and differential thermal analysis, characteristics of TGA and DTA, thermograms, factors affecting TGA and DTA curves, instrumentation, applications of thermogravimetry, applications of DTA, thermometric titration, electrogravimetry, principle and applications.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, 9th Ed., Brooks Cole, 2013.
2. G. D. Christian, *Analytical Chemistry*, 6th Ed., Wiley, 2007.
3. D. A. Skoog, F. J. Holler and S. R. Crouch, *Principles of Instrumental Analysis*, Thomson Learning, 2007.
4. H. H. Willard, L. Jr. Merritt., J. A. Dean and F. A. Settle, *Instrumental Methods of Analysis*, 7th Ed., CBS Publishers, 2007.
5. R.M. Verma, *Analytical Chemistry Theory and Practice*, 3rd Ed., CBS Publishers, 1994.
6. B. K. Sharma, *Instrumental Methods of Analysis*, 28th Ed., GOEL Publishing House, 2012.
7. N. Gray, M. Calvin and S.C. Bhatia, *Instrumental Methods of Analysis*, CBS Publishers, 2009.

8. R.S. Khandpur, *Handbook of Analytical Instruments*, 2nd Ed., Tata McGraw-Hill 2010.
Unit-I: (Skoog) (Christian) (Verma) (Khandpur)
Unit-II: (Skoog) (Sharma)
Unit-III: (Skoog)(Willard) (Gray) (Sharma)
Unit-IV: (Christian) (Khandpur)
Unit-V: (Christian) (Willard) (Khandpur)

References

1. J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education,2007.
2. R. D. Braun, *Introduction to Instrumental Analysis*, PharmaMed Press, 2009.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

MAJOR ELECTIVES II

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY4EA	Bioorganic Chemistry	3	1	-	1	4	4

Instructional objectives	At the end of this course the learner is expected:	Student Outcomes				
1.	To understand the organic chemistry of biomolecules like amino acids, peptides, nucleic acids and carbohydrates.	a	b			
2.	To learn about how enzymes and coenzymes work.			c	d	g

Unit – I Aminoacids, peptides and proteins

Amino acids: acid base properties, isoelectric point, separation, resolution of racemic mixtures of amino acids, asymmetric synthesis

Peptide bonds: peptide secondary structures and their stabilization, strategies for peptide synthesis, automated peptide synthesis.

Proteins: primary, secondary, tertiary and quaternary structures, protein denaturation, natural β-amino acids and β-peptides; β-turn peptidomimetics, β-lactam based peptidomimetics.

Unit – II Enzymes

Classification of enzymes, enzyme catalysis and kinetics, nucleophilic, acid, base and metal-ion catalysis, the catalytic triad, mechanisms of carboxypeptidase A, serine proteases and lysozyme, enzyme inhibition and drug design, enzymes in organic synthesis; antibody catalyzed organic reactions.

Unit – III Organic chemistry of coenzymes

Niacin and its role in redox reactions, mechanisms for pyridine nucleotide coenzymes, flavin adenine dinucleotide and flavin mononucleotide, mechanisms for flavin nucleotide coenzymes, thiamine pyrophosphate and its role in the pyruvate decarboxylase mechanism, biotin and its role in the pyruvate decarboxylase system, pyridoxal phosphate and its role in decarboxylation, transamination, racemization of amino acids, C-C bond cleavage and α,β-elimination.

Unit – IV Bioorganic chemistry of nucleic acids

Nucleic acids: nucleosides and nucleotides, conformation of sugar-phosphate backbone, hydrogen bonding by bases, the double helix,A, B, and Z double helices, stability of double helix, replication, transcription and translation, DNA intercalators, chemical synthesis of DNA, catalytic RNA, siRNA, micro RNA, synthesis and applications of unnatural nucleosides, fluorescently labeled nucleosides and oligonucleotide probes, homogeneous DNA detection, microarray based DNA detection, basics of peptide nucleic acids.

Unit – V Carbohydrates

Classification of carbohydrates, configuration, redox reactions of monosaccharides, Kiliani-Fischer synthesis, Ruff degradation, hemiacetals and cyclic structure of monosaccharides, glycosides, anomeric effect, reducing and non-reducing sugars, disaccharides and polysaccharides.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. P. Y. Bruice, *Organic Chemistry*, 5th Ed., Pearson, 2014.
2. D.V.Vranken and G.A. Weiss, *Introduction to Bioorganic Chemistry and Chemical Biology*, 1st Ed., Garland Science, 2012.
3. T. K. Lindhorst, *Essentials of Carbohydrate Chemistry and Biochemistry*, 3rd Ed., Wiley 2007.
4. N. Sewald and H.D Jakubke, *Peptides: Chemistry and Biology*, 2nd Ed. Wiley, 2009.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

Course Code	**Course Title**	**L**	**T**	**P**	**O**	**L+T+P**	**C**
18PCY4EB	**Materials Chemistry**	**3**	**1**	**-**	**1**	**4**	**4**

Instructional objectives At the end of this course the learner is expected:		**Student Outcomes**				
1.	To understand the basics of crystalline and amorphous materials.	a	b	c		
2.	To learn about nanomaterials.	a	b			g
3.	To learn the basic principles of material characterisation.	a			d	g

Unit – I Crystalline materials

Fundamentals of lattice, unit cell, atomic coordinate, Bravais Lattices, crystal's direction and planes, crystal structures, representation of crystal Structures, defects: point, line, surface, bulk,synthetic approaches for crystalline functional materials - chemical and physical methods.

Unit – II Amorphous and electronic materials

Amorphous solid, oxide glasses, chalcogenide glasses, amorphous carbon, graphite, diamond, alkaline graphite, polymer compounds, band theory,metals, insulators and semiconductors,optical properties of materials,band gap, doping and devices.

Unit – III Nanomaterials

Nanomaterials, quantumconfinement and quantum nanostructures, surface energy and surface area of nanomaterials,fabrication methods of nanomaterials, top-down and bottom-up approaches, 0D,1Dand2D nanomaterials,examples and applications.

Unit – IV Properties of materials

Mechanical properties: fractures of metal, ductile fracture, brittle fracture, toughness and impact testing, magnetic properties: para, ferro, anti-ferro and ferri, electrical properties:thermoelectric, dielectric, piezoelectric, pyroelectric and ferroelectric effect.

Unit – V Characterization of materials

Spectroscopic methods: UV-Vis, IR and Raman, X-ray diffraction, electron microscopy: SEM, TEM and XPS, probe analysis: AFM, Instrumentation, basic working principle and examples in analysis for all the above.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. A. R. West, *Basic Solid State Chemistry*, 2nd Ed., John Wiley &Sons Ltd., 1999.
2. K. J. Klabunde, *Nanoscale materials in Chemistry*, Wiley Interscience, New York, 2001
3. C. Giacovazzo,*Fundamentals of Crystallography*, Oxford University Press, 2002.
4. W. D. Callister and D. G. Rethwisch,*Materials Science and Engineering: An Introduction*,9th Ed., Wiley, 2013.
5. D. J. Ward,*Materials Science*, Lerner Classroom, 2008.

Course Nature : Theory								
Assessment Method (Max.Marks: 100)								
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY4EC	Supramolecular Chemistry and Crystal Engineering	3	1	-	1	4	4

Instructional objectives At the end of this course the learner is expected:		Student Outcomes				
1.	To understand the basic ideas of supramolecular chemistry.	a	b	c		
2.	To introduce the student to the emerging field of crystal engineering.	a			d	g

Unit – I Basic concepts

Terminology and nomenclature in supramolecular chemistry, definition of supramolecular chemistry, chemical interactions leading to supramolecular assemblies, nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-pi, anion-pi, pi-pi and Van der Waals interactions.

Unit – II Host-Guest chemistry

Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands, and hemicarcerands, host-guest interactions, pre-organization and complimentarity, lock and key analogy,binding of cationic, anionic, ion pair and neutral guest molecules.

Unit – III Crystal engineering

Crystal engineering: role of H-bonding, halogen bonding and other weak interactions,co-crystals, salts, polymorphs and their physico-chemical properties,coordination polymers, metal organic frameworks and their properties.

Unit – IV Self-Assembly

Self-assembly of molecules: Design, synthesis and properties of the molecules, self assembling by H-bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots, examples of recent developments in supramolecular chemistry.

Unit – V Molecular devices

Molecular devices: Molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic. Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. J.M. Lehn, *Supramolecular Chemistry-Concepts and Perspectives*, Wiley-VCH, 1995.
2. P. D. Beer, P. A. Gale and D. K. Smith, *Supramolecular Chemistry*, Oxford University Press, 1999.
3. J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, 1st Ed., Wiley, 2000.
4. J.W.Steed,*Core Concepts in Supramolecular Chemistry and Nanochemistry*,1stEd., John Wiley & Sons, 2007.
5. J.D. Seader, I. W. Hamley, *Introduction to soft mater Synthetic and Biological self assembly materials, Separation process principles*,2nd Ed.,Wiley, 2010.
6. G. R. Desiraju, J. J. Vittal and A. Ramanan, *Crystal Engineering: A Textbook*, World Scientific, 2011.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

Course Code	**Course Title**	**L**	**T**	**P**	**O**	**L+T+P**	**C**
18PCY4ED	**Special Topics in Organic Synthesis**	**3**	**1**	**-**	**1**	**4**	**4**

Instructional objectives **At the end of this course the learner is expected:**		**Student Outcomes**				
1.	To acquire knowledge about asymmetric synthesis and organocatalysis.	**a**			**d**	**g**
2.	To learn about the applications of enzymes in organic synthesis.	**a**	**b**	**c**		

Unit – I Asymmetric synthesis

Asymmetric synthesis: chiral auxiliaries, methods of asymmetric induction, substrate, reagent and catalyst controlled reactions, determination of enantiomeric and diastereomeric excess, enantio-discrimination, resolution – optical and kinetic, asymmetric oxidation [epoxidation: Sharpless, Jacobsen, Shi), dihydroxylation (Sharpless)], asymmetric reduction (Noyori, Corey, Pfaltz), stereoselective aldol reactions (Cram's rule and Felkin Anh models),auxillary controlled stereoselection: Evans oxazolidones.

Unit – II Organocatalysis-I

Introduction to organocatalysis, Lewis base catalysis, iminium catalysis, enamine catalysis, Lewis acid catalysis, Bronsted acid and base catalysis, examples.

Unit – III Organocatalysis-II

Carbenes as organocatalysts, types of different NHCs and their synthesis, NHC catalyzed umpolung, NHC catalyzed transesterification reactions, homo and cross benzoin type reactions, Stetter reaction, enolate chemistry, homoenolate derived reactions, addition to ketenes and analogs, oxidative NHC catalysis, cooperative catalysis with metal catalysts, cooperative catalysis with otherorganocatalysts.

Unit – IV Biocatalysis in organic synthesis-I

Introduction to biocatalysts, advantages and disadvantages of biocatalysts, isolated enzymes vs. whole cell systems, brief overview of structure of enzymes, mechanistic aspects of enzyme catalysis, classification and nomenclature, coenzymes, enzyme sources, biocatalysed hydrolytic reactions, hydrolysis of amides, esters, epoxides and nitriles, biocatalytic reduction reactions, recycling of cofactors, reduction of aldehydes, ketones and C=C bonds.

Unit – V Biocatalysis in organic synthesis-II

Oxidation reactions, oxidation of alcohols and aldehydes, biocatalytic carbon-carbon bond formations, aldol reaction, Michael-type additions, thiamine-dependant benzoin condensation, cyanohydrin formation, amino transfer reactions, halogenations and dehalogenations, enzymes in organic solvents, ester synthesis, lactone synthesis, amide synthesis, peptide synthesis, artificial enzyme mimics, and catalytic antibodies.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. R. Gawley and J. Aube,*Principles of Asymmetric Synthesis*, 2nd Ed., Elsevier, 2012.
2. K. Faber, *Biotransformations in Organic Chemistry*, 6th Ed., Springer, 2011.

References

1. Seayad, Jayasree, and Benjamin List. "Asymmetric organocatalysis." *Organic & biomolecular chemistry* 3.5 (2005): 719-724.
2. Hopkinson, Matthew N., et al. "An overview of N-heterocyclic carbenes." *Nature* 510.7506 (2014): 485-496.
3. Flanigan, Darrin M., et al. "Organocatalytic reactions enabled by N-heterocyclic carbenes." *Chem. Rev* 115.17 (2015): 9307-9387.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	Assessment Tool	Cycle Test I	Cycle Test II	Model Examination	Assignment	Attendance	Total
	Marks	10	10	20	5	5	50%
End Semester Weightage							50%
Total							100%

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY4EE	Nanomaterials and Nanochemistry	3	1	-	1	4	4

Instructional objectives At the end of this course the learner is expected:		Student Outcomes				
1.	To acquire knowledge about nanochemistry.	a	b	c	d	g
2.	To learn the synthesis of nanomaterials, characterization and applications.			c	d	g

Unit – I Basic concepts of nanochemistry

Introduction to nanoscience and nanotechnology, discussion on various phenomenon at nano-scale, such as size, shape, surface, surface energy, surface stabilization, characteristic length, self-assembly, defects, size quantization, surface plasmon, conductivity, tunneling, magnetism, defects.

Unit – II Synthesis of nanomaterials

Basics of nanofabrication method: top-down, bottom-up approaches, gas phase, liquid phase, solid phase synthesis, self-assembly, templated synthesis, sol-gel, electrodepostion, fundamentals of nanoparticle formation, thermodynamic approach, supersaturation, nucleation, growth, homo vs hetero nucleation.

Synthesis of nanoparticles: metallic, semiconducting, quantum dots, oxides, hybrids, micelles and microemulsion as templates for synthesis. 0D, 1D and 2D nanoparticles, core-shell nanoparticles, special nanoparticles, shaped nanoparticles.

Unit – III Characterization techniques

Discussion on various techniques available for characterizing the nanomaterials for their size, shape, morphology, crystalline phase, oxidation states, textural properties (surface area, pore volume, pore size), thermal stability, light absorption and band gap.

Scanning electron microscope (SEM)&Transmission electron microscope(TEM),X-ray powder diffraction (XRD)&X-ray photoelectron spectroscope (XPS),Scanning tunnelling microscope (STM)and Atomic force microscope (AFM).

Thermal analysis,N_2 sorption techniques for textural properties of the materialsolid state NMR for characterizing functionalized materials.

Unit – IV Carbon clusters and nanostructures

Bonding in carbon, new carbon structures, carbon clusters, discovery of C60,alkali doped C60,superconductivity in C60,larger and smaller fullerenes, carbon nanotubes: synthesis, single walled carbon nanotubes, structure and characterization, mechanism of formation, chemically modified carbon nanotubes, doping, functionalizing nanotubes, application of carbon nanotubes, nanowires, synthetic strategies, gas phase and solution phase growth, growth control, properties.

Unit – V Nanomaterials for catalysis

Nanocatalysis: fundamentals, homogeneous vs heterogeneous catalysis, effect of surface area, effect of particle size, shape and morphology, effect of composition, bimetallic system etc, nanomaterials for photo-catalysis [dye degradation, water splitting, organic transformations, plasmon assisted photo-catalysis, band gap tuning, etc], nanomaterials for CO_2 capture and conversion.

Tutorials: Tutorial sheet with relevant problems will be provided by the Instructor.

Textbooks

1. C. N. R.Rao, A. Muller and A. K. Cheetam, (Eds) (2004): *The Chemistry of Nanomaterials*, Vol.1, and 2, Wiley – VCH, Weinheim.
2. C. P. Poole, and Jr. F. J. Owens,*Introduction to Nanotechnology*, Wiley Interscience, New Jersey. 2003.
3. K. J. Klabunde, *Nanoscale materials in Chemistry*, Wiley- Interscience, New York, 2001.
4. T. Pradeep, *Nano: The Essentials in Understanding Nanoscience and Nanotechnology*, Tata McGraw Hill, New Delhi, 2007.
5. T. Tang and P. Sheng, *Nano Science and Technology – Novel Structures and Phenomena*, Taylor & Francis, New York, 2004.
6. U. Heiz, and U. Landman,*Nanocatalysis, Springer*, New York, 2006.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

Non-Major Electives

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY2NA	**Nanochemistry**	**2**	**-**	**-**	**-**	**2**	**2**

Instructional objectives **At the end of this course the learner is expected:**		**Student Outcomes**				
1.	To acquire knowledge about nanochemistry.	**a**	**b**	**c**		**g**
2.	To learn about the synthesis of nanomaterials, their characterization and applications.	**a**			**d**	**g**

Unit – I Introduction to nanochemistry

Definition of nano dimensional materials, some historical milestones in the saga of nano forms, size effects, importance of nanomaterials, classification of nanomaterials, simple examples of unique properties of nano sized materials, elementary aspects of bio nanotechnology, some important recent discoveries in nanoscience and technology.

Unit – II Techniques in nanochemistry

Techniques for characterisation of nanoscale materials (basic aspects): atomic force microscope (AFM), transmission electron microscope (TEM), resolution and scanning transmission electron microscope (STEM), scanning tunneling microscope (STM), scanning near field optical microscope (SNOM), and surface plasmon spectroscopy.

Unit – III Synthesis of nanomaterials

Chemical methods in preparation of nanomaterials: sol–gel technique, co-precipitation hydrolysis, sonochemical method, combustion technique, colloidal precipitation, template process.

Inorganic nanoparticles and nanoporous materials**:** oxide nanoparticles, oxomolybdates, nano catalysis, porous silicon, transition and non- transition metal phosphates.

Unit – IV Carbon clusters and nanostructures

Nature of carbon bond, new carbon structures, carbon clusters: discovery of C60, alkali doped C60, superconductivity in C60,larger and smaller fullerenes, carbon nanotubes: synthesis, single walled carbon nanotubes, structure and characterization, mechanism of formation, chemically modified carbon nanotubes, doping, functionalizing nanotubes, application of carbon nanotubes, nanowires, synthetic strategies, gas phase and solution phase growth, growth control, properties.

Unit – V Organic films and supramolecular assembly

Organic films, insulating and passivating layers, electron transfer, organic nanostructures, optical properties, organic semiconductors, active organic devices, polymerization, sizes of polymers, nanocrystals, conductive polymers, block co-polymers, supramolecular structures, transition-metal mediated types, dendritic molecules, supramolecular dendrimers, micelles, biological nanostructures, examples of proteins.

Applications of nanomaterials: applications of nanoparticles in fundamental research, industries, medical field and environmental issue, toxicity, biosafety and ethical issues.

Textbooks:

1. C. N. R. Rao, A. Muller and A. K. Cheetam, (Eds) *The Chemistry of Nanomaterials*, Vol.1, and 2, Wiley – VCH, Weinheim, 2004.
2. C. P. Poole, and Jr. F. J. Owens, *Introduction to Nanotechnology*, Wiley Interscience, New Jersey. 2003.
3. K. J. Klabunde, *Nanoscale materials in Chemistry*, Wiley- Interscience, New York, 2001.
4. T. Pradeep, *Nano: The Essentials in Understanding Nanoscience and Nanotechnology*, Tata McGraw Hill, New Delhi, 2007.
5. T. Tang and P. Sheng, *Nano Science and Technology – Novel Structures and Phenomena*, Taylor & Francis, New York, 2004.
6. U. Heiz, and U. Landman, *Nanocatalysis, Springer*, New York, 2006.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	Assessment Tool	Cycle Test I	Cycle Test II	Model Examination	Assignment	Attendance	Total
	Marks	10	10	20	5	5	50%
End Semester Weightage							50%
Total							100%

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY2NB	Electrochemical Energy Systems	2	-	-	-	2	2

Instructional objectives At the end of this course the learner is expected:		Student Outcomes				
1.	To understand the role of electrochemistry in energy systems.	a	b	c	d	
2.	To learn the kinetics and thermodynamics of electrochemical reactions.			c		g

Unit – I Introduction and thermodynamics of electrochemical reactions

Basic physics of galvanic cells, electrochemical energy conversion, electrochemical energy storage, dynamics of equivalent circuits, impedance of electrode, statistical thermodynamics, the Nernst equation, Gibbs free energy, standard electrode potentials, redox reactions, the Fermi potential, thermodynamics of the transfer of ions between two phases and reconstitution electrodes, thermal and electrochemical stability.

Unit – II Kinetics of electrochemical reactions

Faradaic reactions in concentrated solutions, theory of chemical kinetics and charge transfer based on nonequilibrium thermodynamics, Butler-Volmer equation, electrocatalysis, ion adsorption and intercalation, electrochemical phase transformations, charge transfer at metal electrodes, electrode-electrolytes interfacial/surface studies, charge transfer kinetics at the solid/solid interface in porous electrodes, mass transfer kinetics, transient diffusion, charge diffusion in electrolytes, charge transport in bulk electrolytes.

Unit – III Transport phenomena

Concentration polarization, activation polarization, ion concentration polarization, solution impedance, charge transfer impedance, Warburg impedance percolation, porous electrodes for batteries and supercapacitors, non-equilibrium thermodynamics of porous electrodes, properties of aqueous electrolytes, organic electrolytes, ionic liquid electrolytes, solid electrolytes.

Unit – IV Electrochemical analytical techniques

Cyclicvoltammetry, electrochemical impedance spectroscopy, chrono-amperometry/potentiometry, scanning electrochemical microscopy.

Unit – V Energy storage and conversion devices

Charge storage mechanism**,** lead-acid batteries**,** metal ion batteries, metal sulfur batteries, metal air batteries**,** supercapacitors**,** pesudocapacitors**,** fuel cells, advanced Li-ion and beyond Li-ion battery systems (multivalent battery systems), redox-flow batteries, solid state thin film batteries, solid state micro supercapacitors.

Textbooks

1. C**. Breitkopf**and K.**Swider-Lyons**, (Eds.) *Springer Handbook of Electrochemical Energy,* Springer, 2017.
2. J. Newman, E. Karen Thomas-Alyea, *Electrochemical Systems*. 3rd Ed.,Wiley-Interscience, 2004.
3. O' Hayre, Ryan, Suk-Won Cha, et al. *Fuel Cell Fundamentals*. 2nd Ed., Wiley, 2009.
4. A.*J. Bard and L.R. Faulkner, Electrochemical Methods: Fundamentals and Applications.* 2nd Ed.,Wiley, 2001.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	Assessment Tool	Cycle Test I	Cycle Test II	Model Examination	Assignment	Attendance	Total
	Marks	10	10	20	5	5	50%
End Semester Weightage							50%
Total							100%

Course Code	Course Title	L	T	P	O	L+T+P	C
18PCY3NA	Chemistry of Biomolecules	2	0	0	0	2	2

Instructional objectives At the end of this course the learner is expected:		Student Outcomes				
1.	To get a basic understanding about the chemistry of biomolecules like amino acids, proteins, nucleic acids, lipids and carbohydrates.	a			d	g
2.	To appreciate the role of these biomolecules in biology.	a	b	c		

Unit – I Amino acids and proteins

Classification and structure of amino acids, configuration of amino acids, acid-base properties and isoelectric point, separation of amino acids, peptide bonds, disulfide linkages, proteins classification based on solubility, shape, composition and function, structure of proteins, determination of the primary structure of a protein, secondary, tertiary and quaternary structures, protein denaturation.

Unit – II Enzymes, co-enzymes and their mechanism of action

Enzymes, Classification, kinetics, inhibition, mechanisms of enzyme action, cofactors as derived from vitamins, co-enzymes, prosthetic, prosthetic group and apoenzymes, structure and biological functions of coenzyme-A, thiamine pyrophosphate, pyridoxal phosphate, NAD+, NADP+, FAD, lipoic acid, overview of reactions catalysed by the above cofactors.

Unit – III Nucleic acids

Nature of genetic material, structure of purine and pyrimidine, nucleotides and nucleosides, types of nucleic acids, structure of DNA, properties of nucleic acids, -Tm, denaturation and renaturation, hypo and hyperchromicity, basic ideas on replication, transcription and translation, determination of the base sequence of DNA.

Unit – IV Lipids

Fatty acids classification, nomenclature, structure and properties of fatty acids - structure and function of prostaglandins, tri-acyl glycerol, structure and functions of phospholipids, spingomyelin, plasmologens, structure and function of glycolipids, cholesterol.

Unit – V Carbohydrates

Classification of carbohydrates, stereo isomerism and optical isomerism of sugars, mutarotation, occurrence, structure and biological importance of mono, di and polysaccharides, an introduction to mucopolysaccharides, reactions of carbohydrates due to the presence of hydroxyl, aldehyde and ketone groups.

Textbooks

1. D. L. Nelson, M. M. Cox, *Lehninger Principles of Biochemistry*, 5thEd., W. H. Freeman; New York, USA, 2005.
2. R. K. Murray, D. K. Grammer, *Harper's Biochemistry,* 29th Ed., McGraw Hill, Lange Medical Books, United Kingdom, 2009.
3. J.L. Jain, S. Jain, N. Jain, *Fundamentals of Biochemistry*, S. Chand & Company. India, 2013.
4. P. Y. Bruice, *Organic Chemistry*, 5th Ed., Pearson, 2014.

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**

Course Code	**Course Title**	**L**	**T**	**P**	**O**	**L+T+P**	**C**
18PCY3NB	**Forensic Science**	**2**	**-**	**-**	**-**	**2**	**2**

Instructional objectives	**At the end of this course the learner is expected:**	**Student Outcomes**				
1.	To introduce the student to the basic ideas in forensic science.	**a**	**b**	**c**		
2.	To familiarize the student with chemical and biological techniques used in forensic science.	**a**			**d**	**g**

Unit – I Forensic chemistry

Introduction to forensic science, development of forensic science and criminal prosecution in India, forensic science and victims: Indian scenario, forensic chemistry, theory of forensic analysis, fingerprint development, presumptive drug analysis, soil analysis, thin layer chromatography and ink analysis: introduction, examination process, analysis, clandestine drug laboratories.

Unit – II The history of forensic chemistry and chemical analysis

Introduction, some important techniques of forensic chemistry (trace evidence, fingerprinting, testing for alcohol, serology, bloodstain pattern analysis, fire debris analysis, toxicology),the role of analytical chemistry in forensic science (laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS), alternative light photography, high-speed ballistics photography, video spectral comparator 2000, digital surveillance for xbox (XFT device), 3D forensic facial reconstruction, DNA sequencer, forensic carbon-14 dating, magnetic fingerprinting and automated fingerprint identification (AFIS), high-performance liquid chromatography, gas chromatography, ion chromatography)

Unit – III Forensic biology: serology and DNA testing

Introduction, types of evidence examined, planning the examination, evidence processing, note taking, and report writing, serology testing, identification of blood, identification of saliva.

Unit – IV Forensic biology: DNA testing

DNA testing, combined DNA index system (CODIS) database, DNA in criminal proceedings, sample processing, quality assurance, laboratory accreditation, educational requirements for forensic biology personnel, proficiency testing.

Unit – V Polygraph test and its legal implication in the Indian criminal justice system

Introduction, brief history, application and utility, procedure of interrogation and questioning to the subject, legal status of polygraph, rights of the subject, NHRC's guidelines on administration of lie detector or polygraph test.

Textbooks

1. D. Collins, *Forensic Chemistry*, Brigham Young University – Idaho, 2006.
2. L. Gefrides and K. Welch, *The Forensic Laboratory Handbook, Procedures and Practice*, Springer Science+Business Media, 2011.

References

1. M. G. Tarase, D. H. Prakash, and M. S. Ramadurg. "*Scientific and legal procedure of polygraph test.*"
2. N. Grover and I. Tyagi, *International Journal of Scientific and Research Publications*, Volume 4, Issue 12, December 2012.
3. R. K. Jena*, International Journal of Applied Research,* 2017; 3(2): 283-287.
4. M. Barar, *International Journal of MediPharm Research,* 2016; 2(1),pp 10-16

Course Nature : Theory							
Assessment Method (Max.Marks: 100)							
In Semester	**Assessment Tool**	**Cycle Test I**	**Cycle Test II**	**Model Examination**	**Assignment**	**Attendance**	**Total**
	Marks	**10**	**10**	**20**	**5**	**5**	**50%**
End Semester Weightage							**50%**
Total							**100%**