Course Name : Master of Science
Discipline : Chemistry

Course Objective:

1. To provide adequate knowledge of various chemical phenomena including the recent developments in Chemistry.
2. To instill the confidence in the students to do independent research work.
3. To ensure an excellent knowledge of applications in Chemistry.
4. To enable the students to get employed in the emerging fields of environmental chemistry, food preservation techniques and also in other thrust fields of chemistry.

Eligibility for admission:

The candidates should have a Bachelor Degree in Chemistry from Madurai Kamaraj University or from any other University recognized by the syndicate of Madurai Kamaraj University.

Duration of the course:

Two years

Medium of Instruction and Examination:

The medium of instruction as well as the examination will be English.

Course scheme:

Sem	Part	Subject	Hr	Cr	Int+Ext = Total	Code
I	III	Core Subject I – Organic chemistry I	5	4	25+75= 100	P1CHC11
	III	Core Subject II – Inorganic chemistry I	5	4	25+75= 100	P1CHC12
	III	Core Subject III – Physical chemistry I	5	4	25+75= 100	P1CHC13
	III	Core lab I – Organic chemistry practical I	4	-	---	---
	III	Core lab II – Inorganic chemistry practical I	4	-	---	---
	III	Core lab III – Physical chemistry practical I	3	-	---	---
	III	Major Elective 1 – Computational chemistry/ Biochemistry	4	4	25+75= 100	P1CHE11/ P1CHE12
II	III	Core Subject IV – Organic chemistry II	5	4	25+75= 100	P1CHC21
	III	Core Subject V – Inorganic chemistry II	5	4	25+75= 100	P1CHC22
	III	Core Subject VI – Physical chemistry II	5	4	25+75= 100	P1CHC23
	III	Core lab I – Organic chemistry practical I	4	4	40+60 =100	P1CHC2P1

	III	Core lab II – Inorganic chemistry practical I	4	4	40+60 =100	P1CHC2P2
	III	Core lab III – Physical chemistry practical I	3	3	40+60 =100	P1CHC2P3
	III	Non-Major Elective – Industrial chemistry/ Forensic Science and Crime Investigation	4	4	25+75= 100	P1CHN21/ P1CHN22

Semester II – Part IV – Non-Major Elective – Forensic Science and Crime Investigation

Hours per week: 4 **Credits: 4**

Subject Code: P1CHN22

Unit 1: Introduction to forensic science

Forensic science: Definition, principles and uses in crime investigation, criminology and penology – definition. Finger prints – definitions, important features, patterns, classification, chance prints – visible, plastic and latent prints – development of latent prints – physical and chemical methods, identification of finger prints.

Unit 2: Tracks and traces

Tracks and traces – footprints – nature, location, collection of foot prints, residue prints, walking pattern or tyre marks, tool marks, glass fracture, paints, fibers and police dogs

Unit 3: Poisons

Poisons- classification, diagnosis of poisoning (Arsenic, cyanide, opium and snake) in the living and in dead – clinical symptoms, postmortem appearances – use of antidotes for common poisons (acid, alkali, mercury and snake).

Unit 4: Analysis of biological substances

Analysis of biological substances in crime investigation – blood, semen, saliva, urine and hair – cranial analysis (head and teeth) – DNA finger printing for tissue identification in disembered bodies – detecting steroid consumption in athletes. Incendiary and timed bombs in road and railway tracks – defusing live bombs.

Unit 5: Documents

Documents – different types of forged signatures – simulated and traced forgeries using ultraviolet rays, comparison of typewritten letters, checking silver line and water mark in currency notes, types of counterfeit coins, AAS analysis to detect counterfeit coins, gold purity in 22 carat ornaments and authenticity of diamond

Reference books

1. R.Saferstein, Criminalities and Introduction to Forensic Science, Prentice Hall of India, 1978.
2. C.K.Sinha, Pankaj Kumar and Prashant Jha, Forensic Medicine and Toxicology, 6th edition, Scientific Book Company, Patna, 2007.

Semester-I- Part –III- Core Subject I- Organic Chemistry I

Hours per week: 5 **Credits: 4**

Subject Code: P1CHC11

Unit I: Electron displacement and structure – reactivity correlation **12 Hours**

Inductive and field effects – bond distances – bond energies – delocalized bonds – cross conjugation – rules of resonance – resonance energy – resonance effect – steric inhibition of resonance – Hyperconjugation – hydrogen bonding – effect of structure on the dissociation constants of acids and bases – HASB concepts.

Quantitative treatment of the effect of structure on reactivity – The Hammett relationship – significance of reaction and substituent constants – application of the Hammett equation in reaction mechanism – limitations and deviations.

Unit II: Introduction to reaction mechanism **12 Hours**

Reaction intermediates – free radicals, carbenes, nitrenes, carbanions, carbocations – formation and stability of reaction intermediates – methods of determination of reaction mechanism – kinetic and thermodynamic control of chemical reactions. Kinetic and non-kinetic methods for determining organic reaction mechanism – principle of microscopic reversibility – energy profile diagram – Hammond postulate.

Unit III: Stereochemistry **12 Hours**

Concept of chirality, necessary and sufficient conditions for chirality – relationship between substrate symmetry and chirality. Projection formulae – Wedge, Fischer, Sawhorse and Newmann. Optical isomerism due to centre of chirality. Molecules with one stereogenic centre (chiral centre) and molecules with more than one chiral centre. Erythro and threo nomenclature. Configuration – determination of configuration. Cahn, Ingold and Prelog system (R-S) of designation of configuration.

Geometrical isomerism

E-Z nomenclature – determination of configuration of geometrical isomers using physical and chemical methods – stereoisomerism in monocyclic compounds (upto six membered ring).

Prochirality and prostereoisomerism , enantiotopic and diasterotopic ligands and faces and their nomenclature – pro-R and pro-S and Re and Si faces, Stereospecific and stereoselective reactions. Asymmetric synthesis; Cram and Prelog rules. Optical isomerism due to axial chirality – biphenyls, allenes and spiranes. Molecules with planar chirality – paracyclophanes, trans cyclooctene, ansa compounds.

Unit IV: Aromatic character **12 Hours**

Aromatic character in benzene, six membered rings, five, seven and eight membered rings – other systems with aromatic sextets – Huckel's rule – Craig's rule – concept of homoaromaticity and antiaromaticity – systems with 2,4,8 and 10 electrons – systems with more than 10 electron – Alternant and nonalternant hydrocarbons. Chemistry of cyclopentadienyl anion – Fulvene, Azulene, Tropolones, Sydnones and Annulenes.

Novel ring systems

Nomenclature of bicyclic and tricyclic systems – chemistry of adamentane, diamantane (congressane), cubane and catenanes.

Unit V: Spectroscopy I **12 Hours**

UV Spectroscopy : Principle – absorption spectra of conjugated dienes – α,β-unsaturated carbonyl compounds – Woodward–Fieser rules.

IR Spectroscopy: Molecular vibrations – vibrational frequency – factors influencing group frequencies – quantitative studies.

Mass Spectroscopy: Principle – type of ions – base peak – parent ion , metastable and isotopic peaks – fragmentation – general rules – pattern of fragmentation for various classes of compounds – McLafferty rearrangement – Retro Diels – Alder reaction.

Reference books

1. P.Sykes, Guidebook to Mechanism in Organic Chemistry, Orient Longmann Ltd., New Delhi,
1998.
2. Jerry March, Advanced Organic Chemistry , John Wiley and Sons, 4th edition, 2004.
3. E.S. Gould, Mechanism and Structure of Organic Chemistry, Holt, Rinehart and Winston Inc,
New York, 1959.
4. J. Shorter, Correlation Analysis in Organic Chemistry, Clarendon Press, Oxford, 1973.
5. R.T. Morrison and R.N. Boyd , Organic Chemistry, Prentice – Hall, 6th edition, 2001.
6. I.L Finar, Organic Chemistry Vol. I and II , 6th edition, John Wiley and Sons, New York, 2000.
7. Lowry and K.S. Richardson , Mechanism and Theory in Organic Chemistry.
8. Reinhard Bruckner, Advanced Organic Chemistry, Reaction Mechanisms, Academic Press, 2002.
9. F.A Carey and R.J. Sundberg , Advanced Organic Chemistry, Part B, 5th edition, Springer
Publishers, 2008.
10. William Kemp, Organic Spectroscopy , ELBS , 3rd edition,
11. John R.Dyer, Application of Absorption Spectroscopy of Organic Compounds, 3rd edition,
ELBS, 1987.
12. Robert M.Silverstein and Francis X.Webster, Spectrometric Identification of Organic Compounds, 6th edition, Wiley and Sons, Inc, 2010.
13. P.S.Kalsi, Spectroscopy of Organic Compounds, 6th edition, New Age International Publishers, 2009.
14. Jag Mohan, Organic Analytical Chemistry – Theory and Practice, Narosa Publishing House,
2003.
15. Jag Mohan, Organic Spectroscopy, Principles and Applications, 2nd edition, Narosa Publishing
House, 2010.

Semester-I- Part –III- Core Subject II- Inorganic Chemistry I

Hours per week: 5 **Credits: 4**

Subject Code: P1CHC12

Unit I: Bonding theory 15 Hours

Qualitative treatment of VB and MO theories – σ and π bonds – hybridization and resonance – MO equivalent of hybridization – application of VB and MO theories to the structures of homonuclear and heteronuclear diatomic and triatomic molecules – comparison of VB and MO theories – the concept of multicentre bond as applied to electron deficient molecules – boron hydrides, metal alkyls – VSEPR theory – bonding in xenon compounds.

Unit II: Bond properties and ionic bonding 15 Hours

Bond order, bond energy, bond length – bond polarity – partial ionic character – electronegativity – electron affinity – lattice energy – Born Haber cycle – covalent character in ionic compounds – different types of electrostatic interactions – hydrogen bond – ionic radius –covalent radius – van der Waals radius.

Unit III: Inorganic chains, rings and cages **15 Hours**

Polyacids – classification – isopoly acids like polymolybdate, polyvanadate and polytungstate – their structures – heteropolyacids 12A, 12B, 9 and 6 heteropolyacids – preparation and structure. Phosphazenes and their polymers – phosphonitrilic compounds – S_4N_4 – polymeric sulphur nitride (polythiazyl) cage compound. Boranes – nomenclature of boranes and carboranes –Wade' rules – Styx number – preparation and structures of B_4H_{10} and $C_2B_{10}H_{12}$ – borazine.

Unit IV: Metallurgy **15 Hours**

Occurrence, isolation, purification, properties and uses of the following metals as well as their important compounds: Ti, Zr, V, U, Be, Th, Ge and platimum metals.

Unit V: Co-ordination chemistry I **15 Hours**

IUPAC nomenclature of co-ordination compounds – isomerism in co-ordination compounds – types of ligands – monodentate, ambidentate and macrocyclic ligands – chelate and its applications – detection of complex formation in solution – factors affecting stability constant in solution – determination of stability constant by spectrophotometric, polorographic and potentiometric methods – VB theory of metal complexes.

Reference books

1. J.E.Huheey, E.A.Keiter, R.L.Keiter and O.K.Medhi**,** Inorganic Chemistry: Principles of Structure and Reactivity, 4th edition, Pearson Education Inc., 2006.
2. F.A.Cotton and G.Wilkinson, Advanced Inorganic Chemistry, 6th edition, John Wiley and Sons, New York, 2009.
3. J.D. Lee, Concise Inorganic Chemistry, 5th edition, Blackwell Science Ltd., Oxford, 2000.
4. D.F.Shriver and P.W.Atkins, Inorganic Chemistry, 4th edition, Oxford Univ. Press, 2009.
5. H.D. Mathur and O.P.Tandon, Chemistry of Rare Elements, 3rd edition, S.Chand and Co., 1989.

Semester I – Part III – Core Subject III – Physical Chemistry I

Hours per week: 5 **Credits: 4**

Subject Code: P1CHC13

Unit I: Quantum mechanics –An introduction **15 Hours**

Inadequacy of classical mechanics – Planck's explanation about black-body radiation – de-Broglie's concept of matter waves – distinction between matter waves and electromagnetic radiation – experimental verification of matter waves – Compton effect – Heisenberg's uncertainty principle – Hypothetical (gedenkan) experiments of Heisenberg – Bohr's complementarity principle

Postulates of quantum mechanics – Operator algebra: Expressions – addition, subtraction and multiplication – linear operators – Laplacian operator – vector operator – ladder operator – quantum mechanical operator for the following observables: position, momentum, kinetic energy, potential energy, total energy and angular momentum – commutator algebra – evaluation of commutators – commutation rule for angular momentum – Hermitian operator – properties of Hermitian operator – unitary operator – permutation operator – properties of wave functions – Eigen function – Eigen value – Concept of orthoganality and normalization – significance of ψ and ψ^2.

Unit II: Application of quantum mechanics to simple systems **15 Hours**

Derivation of Schrodinger wave equation – application of SWE to simple systems – Particle in one dimensional box – physical interpretation of the solution of one dimensional box problem such as characteristics of wave function, probability of a particle, component of momentum, uncertainty principle through one dimensional box and electronic transition selection rule – particle moving in three dimensional box – concept of degeneracy and distortion – Particle moving in a ring – Rigid rotator – reduced mass – moment of inertia – rotational energy levels – Simple harmonic oscillator – force constant – zero point energy – Hermite polynomials – Hydrogen atom problem – radial wave function.

Unit III: Application of chemical thermodynamics **15 Hours**

Combining first and second law of thermodynamics – developing fundamental equation of states – Maxwell relations – properties of Gibbs function – temperature dependence of the Gibbs function – Gibbs-Helmholtz equation – the pressure dependence of the Gibbs function – Clausius-Clapeyron equation – derivation and applications – thermodynamics of ideal solutions – free energy change of mixing and entropy changes of mixing – relation between osmotic pressure and vapour pressure lowering – thermodynamic derivation – relation between the depression of freezing point and concentration – elevation of boiling point and concentration.

Unit IV: Chemical and Phase equilibria **15 Hours**

Reaction free energy – reaction isotherm and direction of spontaneity – standard reaction free energy – calculation from thermochemical, electrochemical and equilibrium data – temperature coefficient of reaction free energy and equilibrium constant – temperature and pressure dependence of thermodynamic quantities – thermodynamic explanation of Le Chatelier principle.

Gibbs phase rule – its thermodynamic derivation – application of phase rule to three component systems – formation of one pair, two pairs and three pairs of partially miscible liquids – systems composed of two solids and a liquid.

Unit V: Chemical kinetics I **15 Hours**

Empirical rate laws – influence of temperature on the rate of reaction – Arrhenius rate equation – measurement of thermodynamic parameters – complex reactions – Steady State Approximation – theory of reaction rates – bimolecular collision theory and Absolute Reaction Rate Theory(ARRT). Potential energy surfaces – chain reactions – H_2-Br_2 reaction, decomposition of acetaldehyde, decomposition of N_2O_5, H_2-O_2 explosive reactions.

Unimolecular reaction rate theories – the simple Lindemann treatment – Hinshelwood's theory – Rice, Ramsperger and Kassel (RRK) theory – Marcus theory – Slater's theory – Kinetic isotope effect – reactions in solutions – influence of solvent dielectric constant, effect of ionic strength – Bronsted-Bjerrum equation – primary and secondary salt effect – effect of pressure on reaction rates – significance of volume of activation.

Suggested Readings

1. D.A. McQuarrie, Quantum Chemistry, 1st Indian edition, Viva Books (P) Ltd., New Delhi, 2003.
2. A.K. Chandra, Introductory Quantum Chemistry, 4th edition, Tata-McGraw Hill Pub. Co., New Delhi, 2033.

3. H.W. Hanna, Quantum Mechanics in Chemistry, Benjamin / Cummings Pub. Co., London, 1983.
4. I.N. Levine, Quantum Chemistry, 4th edition, Prentice-Hall India, New Delhi, 2000.
5. D.A. McQuarrie and J.D. Simon, Physical Chemistry - A Molecular Approach, Viva Books (P) Ltd., New Delhi, 2010.
6. S.Glasstone, Thermodynamics for Chemists, East-West Press Private Ltd., New Delhi, 1969.
7. J.Rajaram and J.C.Kuriakose, Thermodynamics, 3rd edition, S.Chand & Co. Ltd., 1986.
8. B.R.Puri, L.R.Sharma and M.S.Pathania, Principles of Physical Chemistry, Millenium Edition, Vishal Publishing Co., Jalandar, 2005.
9. K.J.Laidler, Chemical Kinetics, 3rd edition, Pearson Education, 1987.
10. K.J.Laidler, Theories of Chemical Reaction Rates, McGraw Hill Book Co., London, 1969.

Semester-I- Part – III – Major Elective – Computational Chemistry

Hours per week: 4 **Credits: 4**

Subject Code: P1CHE11

Unit I: Introduction to computational chemistry **12 Hours**

Introduction – tools of computational chemistry – potential energy surface – one dimensional – two dimensional – stationary points – intrinsic reaction coordinate (IRC) – Born Oppenheimer approximation – geometry optimization – Hessian matrix – Eigen vector and value matrices – normal mode vibrations – zero point energy.

Unit II: Molecular mechanics **12 Hours**

Molecular mechanics – developing and parameterizing a force field – bond stretching – angle bending – torsional term – non bonded interactions – calculation using force field – geometries and energies of small to medium sized molecules – geometries and energies of polymers – molecular mechanics in organic synthesis.

Unit III: Ab initio calculations **12 Hours**

Ab initio calculations – basic principles of the ab initio method – Hartree Self Consistent Field (SCF) – method – Hartree Fock (HF) equations – Slater determinants – calculating the atomic-molecular energy – variation theorem – minimizing the energy – basis sets – Gaussian function – types of basis sets and their uses (STO-3G and STO-3G*) – basics of density functional theory (DFT).

Unit IV: Applications of ab initio methods **12 Hours**

Applications of ab initio methods – geometry – energies – calculating quantities relevant to thermodynamics and to kinetics – G2 method and its variants – calculating heats of formation – frequencies of IR bands – intensities of IR bands – dipole moments.

Unit V: Semiempirical methods **12 Hours**

Semiempirical methods – introduction – basic principles of self consistent field semiempirical methods – Pariser-Parr-Pople (PPP) method – Complete Neglect of Differential Overlap (CNDO) method – Neglect of Diatomic Differential Overlap (NDDO) method – Intermediate Neglect of Differential Overlap (INDO) method – heats of formation from semiempirical electronic energies – Modified Neglect of Diatomic Differential Overlap (MNDO) method – Austin Method 1 (AM1) – Parameterized Model number 3 (PM3) method – Semi Ab initio Method number 1 (SAM1) – inclusion of d-orbitals: MNDO/d and PM3t.

References:

1. Computational Chemistry: Introduction to the theory and applications of Molecular and

Quantum Mechanics, Errol Lewars, Springer Publisher, New Delhi, 2008.
2. Principles of Physical Chemistry, Puri, Sharma, Pathania, Vishal Publishing Co., Jalandar.
3. Physical Chemistry, Peter Atkins and Julio de paula, 8th edition, Oxford University Press,
2010.

Semester I – Part III – Major Elective – Biochemistry

Hours per week: 4 **Credits 4**

Subject Code: P1CHE12

Unit I: Enzymes **12 Hours**

Classification, nomenclature, properties of enzymes, some features of active sites of enzymes, enzyme kinetics – Michaelis-Menten model – significance of K_m and V_{max} values. Enzyme inhibition – competitive and noncompetitive inhibitive. Allosteric interaction – mechanism of enzyme action. Lysozyme and carboxypeptidase.

Unit II: Generation and storage of metabolic energy **12 Hours**

Metabolism – basic concepts and design: glycolysis – Citric acid cycle – oxidative phosphorylation – pentose pathway and gluconogenesis. Glycogen and disaccharide metabolism, fatty acid metabolism – amino acid degradation and urea cycle – photosynthesis.

Unit III: Information, storage, transmission, expression of genetic information **12 Hours**

DNA – Genetic role structure and replication: messenger RNA – transcription genetic code and gene protein relationship – protein synthesis, control of gene expression – Eucaryotic chromosomes, recombinant DNA technology and viruses.

Unit IV: Bioinorganic chemistry **12 Hours**

Metalloproteins and enzymes – blue copper proteins – copper proteins as oxidases/ reductases – nickel containing enzymes – structure of DNA – types of nucleic acid interactions – coordination, intercalation and hydrogen bonding – interactions of metal ions with nucleic acid – redox chemistry, hydrolytic chemistry – monitoring the DNA binding by UV, IR, NMR and CV spectral techniques.

Unit V: Biophysical aspects **12 Hours**

Electron transport and oxidative phosphorylation – thermodynamic and kinetic aspects –photosynthesis – an overview – photosystem II – the light harvesting chlorophyll – protein complexes of photosystem II – role of carotenoids in photo synthesis – the primary electron donor of photosystem II, P680 – the stable primary electron acceptor Q_A and the secondary electron acceptor Q_B – the transient intermediate electron of photosystem II – Pheophytin – oxygen evolution – the role of manganese – the electron donor to $P680^+$ – charge recombination in photosystem II – photosystem I light – harvesting chlorophyll – protein complexes of photo system I – the primary electron donor of photo system I, P700 – the primary electron acceptor A_o of photosystem I – the intermediate electron acceptor A_1 of photosystem I – mobile electron carriers plastocyanin and ferredoxin and $NADP^+$ – reductase.

Reference books

1. B.D.Hames and N.M.Hooper , Biochemistry, Viva Books Pvt. Ltd., 2003.
2. J.M.Berg, J.L.Tymoczko and L.Stryer, Biochemistry , V edition, W.H.Freeman and Company, New York, 2002.
3. A.L.Lehninger, Biochemistry, Kalyani Publishers, New Delhi, 1998.
4. D.L.Nelson and M.M.Cox, Lehninger Principles of Biochemistry, 4th edition, W.H.Freeman and Company, New York, 2005.
5. I.Bertini, H.B.Gray, S.J.Lippard and J.S.Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi, 1998.
6. G.R.Chatwal and A.K.Bhagi, Bioinorganic Chemistry, Himalaya Publishing House, 1998.
7. B.Ke, Advances in Photosynthesis, Vol.10, Photosynthesis - Photobiochemistry and Photobiophysics, Kluwer Academic Publishers, Dordrecht, 2001.

Semester II -Part III – Core subject IV –Organic chemistry II

Hours per week : 5 **Cerdits:4**

Subject Code: P1CHC21

Unit I: Conformational analysis **15 Hours**

Configuration and conformation – conformations of ethane and n-butane, 1,2 – dichloroethane – conformation analysis – stereoelectronic and steric factors – conformation of simple acyclic compounds – conformation of cyclohexane and its monosubstituted and disubstituted derivatives – correlation of the conformation of acyclic and cyclic systems with their physical and chemical properties – conformational free energy – Curtin-Hammett principle –quantitative treatment of mobile system – Eliel-Ro equation – conformations and reactivity of cyclohexanones – conformational analysis of aldohexopyranoses.

Unit II: NMR Spectroscopy

^{1}H NMR Spectroscopy **15 Hours**

Origin of NMR Spectra – chemical shift – spin-spin coupling – coupling constant – first and second order spectra – spin-spin splitting – influence of stereochemical factors on chemical shift of protons – simplification of complex spectra – deuterium substitution – spin decoupling – double resonance – shift reagents – Nuclear Overhauser Effect –CIDNP NMR.

^{13}C NMR Spectroscopy **15 Hours**

Basic principle of FT technique – Relaxation time – assignment of signals – Off Resonance Decoupling – additivity relationship – calculation of chemical shifts for aromatic and aliphatic compounds – DEPT ^{13}C-^{13}C correlation COSY and HETCOR.

Composite problems involving UV-Vis, IR, NMR and Mass spectra.

Unit III: Addition to multiple bonds **15 Hours**

Electrophilic, nucleophilic and free radical additions – addition to conjugated systems – orientation of the addendum – stereochemical factors in reactions like addition of hydrogen,halogens, hydrogen halides and hypohalous acids, hydroboration and hydroxylation – epoxidation . Addition to carbonyl groups – mechanism – Aldol condensation – Perkin reaction –Knoevenagel reaction –Mannich reaction – Cannizaro reaction – Benzoin condensation – Claisen ester condensation – Darzen's reaction – Reformatsky reaction – Wittig reaction – Grignard reactions. Addition to α,β-unsaturated carbonyl compounds –

Michael addition – Diels-Alder reaction – addition of carbenes and carbenoids to double and triple bonds. Esterification of acids and hydrolysis of esters – decarboxylation of carboxylic acids.

Unit IV: Aliphatic substitution reactions **15 Hours**

Aliphatic electrophilic substitution

Electrophilic substitution at saturated carbon – S_E1 , S_E2 and S_Ei mechanisms. Aliphatic nucleophilic substitution . Nucleophilicity and basicity – S_N1 and S_N2 mechanisms – effect of substrate structure – effect of attacking nucleophiles, leaving groups and reaction medium – ambident nucleophiles – ambident substrates – neighbouring group participation of n, π and σ electrons – S_Ni mechanism – nucleophilic substitution at an aliphatic trigonal carbon – nucleophilic substitution at an allylic carbon – nucleophilic substitution at a vinyl carbon.

Unit V: Aromatic substitution reactions and elimination reactions **15 Hours**

Aromatic electrophilic substitution – orientation and reactivity – mechanism of nitration, halogenation, Friedel-Craft's reaction and sulphonation – partial rate factors – ortho/para ratio – Quantitative treatment of reactivity of electrophiles (the selectivity relationship) – Aromatic nucleophilic substitution reactions – S_NAr , S_N1 and benzyne mechanisms.

Elimination reactions: α-Elimination, β-elimination, E_1, E_2 and $E1_CB$ mechanism – stereochemistry of elimination – orientation of the double bond – effect of changes in the substrate, base, leaving group and medium on E_1, E_2, $E1_CB$ reactions – elimination *vs* substitution – pyrolytic *cis* elimination – Bredt's rule.

Reference books

1. I.L. Finar, Organic Chemistry, Vol. II, 6th edition, John Wiley and Sons, New York, 2000.
2. T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry.
3. Jerry March, Advanced Organic Chemistry, John Wiley and Sons, 4th edition, 2004.
4. E.S. Gould, Mechanism and Structure of Organic Chemistry, Henry, Rinehart and Winston, New York, 1959.
5. Reinhard Bruckner, Advanced Organic Chemistry , Reaction Mechanisms, Academic press, 2002.
6. F.A.Carey and R.J. Sundberg, Advanced Organic Chemistry, Part B, 5th edition, plenum Publishers, 2008.
7. John R.Dyer, Application of Absorption Spectroscopy of Organic Compounds, 3rd edition,
   ELBS, 1987.
8. William Kemp, Organic Spectroscopy , ELBS , 3rd edition,
9. Robert M.Silverstein, Francis X. Webster, Spectrometric Identification of Organic Compounds, 6th edition, John Wiley and Sons Inc., 2010.
10. P.S.Kalsi, Spectroscopy of Organic Compounds, 6th edition, New Age International Publishers, 2009.
11. Jag Mohan, Organic Analytical Chemistry – Theory and Practice, Narosa Publishing House, 2003.

12. Jag Mohan, Organic Spectroscopy, Principles and Applications, 2nd edition, Narosa Publishing House, 2010.

Semester II – Part III – Core Subject V – Inorganic Chemistry II

Hours per week: 5 **Credits: 4**

Subject Code: P1CHC22

Unit I: Co-ordination Chemistry II **15 Hours**

Theory of bonding – CFT and MO theories – splitting of d-orbitals in Oh, Td, square planar, trigonal bipyramidal and square bipyramidal geometries – tetragonal distortion – Jahn-Teller distortions – CFSE calculation in terms of Dq – factors affecting crystal field splitting – spectrochemical series – application of CFSE – thermodynamic effects of CFSE – MO diagram of octahedral complexes – effect of π-donor and π-acceptor ligands – magnetic properties of transition metal complexes – calculation of spin-only magnetic moments – orbital contribution to the magnetic moment – spin orbit coupling.

Unit II: Complexes of π-acceptor ligands **15 Hours**

Introduction – EAN rule ant its correlation to stability. Synthesis, structure and bonding in metal carbonyls, nitrosyls, complexes and dinitrogen complexes – IR study of metal carbonyls.

Synthesis, properties, structure and bonding in ferrocene, olefin, and allyl complexes – covalent *vs* ionic bonding in beryllocene.

Unit III: Reaction mechanism of co-ordination compounds **15 Hours**

Substitution reactions of octahedral complexes – labile, inert complexes – mechanism of acid hydrolysis – base hydrolysis and anation reaction – substitution reactions of square planar complexes – factors affecting reactivity of square planar complexes – trans-effect and its applications – electron transfer reactions – complementary and non complementary reactions – outer sphere and inner sphere electron transfer mechanism .

Unit IV: Molecular rearrangement reaction of co-ordination complexes **15 Hours**

Molecular rearrangement of four coordinated complexes-six coordinated complexes –reaction at coordinated ligand – reaction due to metal ion polarization of coordinated ligands –hydrolysis of amino acid esters, amides and peptides – aldol condensation – imine formation – the template effect and macrocyclic ligands.

Unit V: Organometallic Catalysis **15 Hours**

Homogeneous catalysis involving organometalics – oxidative addition – reductive elimination – insertion reaction – Wilkinson catalyst, Waker process and hydroformylation. Heterogeneous catalysis – Ziegler-Natta polymerization. Cyclo oligomerisation of acetylenes (Reppe's and Wilkei's catalysis) – carbonylation of alcohols.

Reference books

1. B.N.Figgis, Introduction to Ligand Fields, Interscience Publishers, New York, 1967.
2. K.F. Purcell and J.C. Kotz, Inorganic Chemistry, W.B. Saunders Company, 1977.
3. S.F.A. Kettle, Coordination Compounds, ELBS, 1975.
4. F.Basolo and R.G. Pearson, Mechanism of Inorganic Reaction, A Study of Metal Complexes in Solution, Wiley Eastern, New Delhi,1984.
5. Journal of Chemical Education, March 1986 (for Catalysis).

6. R.Gopalan and V. Ramalingam, Concise Coordination Chemistry, Vikas Publishing House
Pvt. Ltd., New Delhi 2010.

Semester II – Part III – Core Subject VI – Physical Chemistry II

Hours per week: 5 **Credits: 4**

Subject Code: P1CHC23

Unit I: Approximation methods in quantum mechanics **15 Hours**

Radial probability distribution curves and shapes of atomic orbitals – Need for approximation methods – time independent perturbation theory – application to solve the energy of anharmonic oscillator – Helium atom ground state – Linear variation theorem – application to hydrogen atom – He atom – Hatree atomic units – Electron correlation – electron spin and Pauli principle – antisymmetric nature of wave function – Slater determinants – Molecules – Born-Oppenheimer approximation simplifies molecular Hamiltonian operators – VB treatment of hydrogen molecule – coloumbic integral – exchange integral and overlap integral – MO treatment of hydrogen molecular cation, homonuclear and heteronuclear diatomic molecules – Molecular term symbols

Unit II: Fast reaction kinetics and catalysis **15 Hours**

Fast reaction techniques – Chemical relaxation methods, temperature and pressure jump methods, ultrasonic absorption techniques, reaction in flow system, continuous and stopped flow, shock wave tube methods. Chemical kinetics in crossed molecular beams.

Homogeneous catalysis – acid base catalysis – Van't Hoff and Arhenius intermediates for protolytic and prototropic mechanisms. Catalysis in Biological systems – enzyme catalysis – Michaelis–Menten kinetics – Lineweaver and Burk plot – influence of pH on the enzyme catalysis. Heterogeneous catalysis – kinetics and mechanism of unimolecular and bimolecular reactions – Langmuir-Hinshelwood and Langmuir-Rideal mechanism – ARRT of surface reactions – synthesis of ammonia, hydrogenation of ethylene and cracking of hydrocarbons.

Unit III: Introduction to group theory **15 Hours**

Molecular symmetry elements and symmetry operations – various operations with illustrations. Groups and their basic properties – symmetry point group classification – rotational (C), dihedral (D), tetrahedral (Td) and octahedral (Oh) point groups. Order of a group. Classes and similarity transformation – Group multiplication table – cyclic and inverse rule – matrix representation of symmetry operations. Trace or character of the matrix – reducible and irreducible representations – Great orthogonality theorem – construction of character tables – C_{2v}, C_{3v}, C_{4v}, C_{2h} and D_{2d} point groups.

Unit IV: Application of group theory to solve spectroscopic and molecular problems **15 Hours**

Symmetry of normal modes of vibrations: linear and non-linear molecules – physical basis of spectroscopic selection rules – properties of dipole moment, polarizability and definite integrals – IR and Raman active vibrational normal modes of homonuclear and heteronuclear diatomic, linear and non-linear molecules – Mutual exclusion principle with illustration. Prediction of electronic transition selection rules of organic compounds such as formaldehyde, ethylene and benzene – group theoretical prediction of types of hybridization – CH_4, BF_3, $PtCl_4^{2-}$, BF_5 and SF_6.

Unit V: Polymer chemistry **15 Hours**

Overview of polymers – types and properties of polymers – kinetics and mechanism of free radical, ionic and condensation and Zeigler-Natta polymerization processes – emulsion and suspension polymerization techniques. Polymer molecular weight distribution – molecular weight determination – osmotic pressure method – light scattering method – ultracentrifuge method and viscosity method.

Conducting polymers: Introduction – crystallinity of polymers – glass transition temperature – factors affecting the conductivity of conducting polymers – doping of conducting polymers – important structural features – nature of charge carriers in conducting polymers – solitons, polarons and bipolarons.

Reference books

1. D.A.McQuarrie, Quantum Chemistry, 1st Indian Edition, Viva Books (P) Ltd., New Delhi, 2003.
2. A.K.Chandra, Introductory Quantum Chemistry, 3rd Edition, Tata-McGraw Hill Pub. Co., New Delhi, 1988.
3. H.W.Hanna, Quantum Mechanics in Chemistry, Benjamin / Cummings Pub. Co., London, 1983.
4. I.N.Levine, Quantum Chemistry, Allyn and Bacon, Boston, 1983.
5. D.A.McQuarrie and J.D. Simon, Physical Chemistry - A Molecular Approach, Viva Books (P) Ltd., New Delhi, 1998.
6. K.J.Laidler, Chemical Kinetics, 3rd Edition, Pearson Education, 2007.
7. K.J.Laidler, Theories of Chemical Reaction Rates, McGraw Hill Book Co., London 1969.
8. F.A.Cotton, Chemical Applications of Group Theory, 3rd Edition, John Wiley and Sons, New York, 1999.
9. V.Ramakrishnan and M.S.Gopinath, Group Theory in Chemistry, 2nd Edition, Vishal Publications, 1991.
10. K.V. Raman, Group Theory and its Application to Chemistry, Tata McGraw-Hill Pub. Co., 1990.
11. G.Davison, Introduction to Group Theory for Chemist, Applied Sci., Pub., Ltd., London, 1971.
12. R.S. Drago, Physical Methods in Chemistry, W.B. Saunders Co., London, 1977.
13. Fred W.Billmeyer, Textbook of Polymer Science, John Wiley & Sons (Asia) Pte.Ltd.,2007.
14. V.R.Gwariker, N.V.Viswanathan and Jayadev Sreedhar, Polymer Science, New Age International Publishers, New Delhi, 2010.
15. R.J.Young and P.A.Lovell, Introduction to Polymers, 2nd edition, Chapman and Hall, 2000.Anil Kumar and Rakesh K.Gupta, Fundamentals of Polymers, McGraw-Hill Companies Inc., 1998.

Semester II – Part IV – Non-Major Elective – Industrial Chemistry

Hours per week: 4 **Credits: 4**

Subject Code: P1CHN21

Unit 1: Importance of chemical process industry **12 Hours**

Introduction – origin and development of chemical process industry – pre-scientific chemical industry – scientific chemical industry. Growth with restraints – Green challenge to chemical industry – Indian chemical industry today – classification of technologies processes – basic principles of homogeneous and heterogeneous processes.

Unit 2: Raw materials and energy for chemical industry **12 Hours**

Raw materials:

Characteristics of raw materials and their resources – methods of raw material concentration – gravitational benefication – hydroseparator – hydrocyclone – air separator – electromagnetic separation.

Energy for chemical industry: **12 Hours**

Power and Fuels – classification of fuels – coal, fuel gases, Liquid fuels – petroleum cracking

Unit 3: Water conditioning in chemical process industry **12 Hours**

Introduction – sources of water supply – characteristics of water – water for industrial purpose – soft and hard water – softening of water – permutit process – ion exchange process. Types of hardness – disadvantages of using hard water in industry

Unit 4: Small scale chemical industry **12 Hours**

Electroplating: Introduction – factors affecting electroplating – procedure for electroplating. Oils: Classification – fatty oil – essential oil – mineral oils – drying oils – semidrying oils. Waxes: Classification – tests for oils, fats and waxes.

Soaps: Types – hot process – batch process – continuous process – manufacture of soaps by continuous process.

Unit 5: Large scale chemical industry **12 Hours**

Manufacturing process – Raw materials – composition and uses of products in Portland cement – ceramics, rubber, fertilizer, insecticides and pesticides. Photo films industries. Commercial aspects of starting an industry

Reference Books

1. W.V.Mark, Chemical Process Industries, Vol. I and II, 2nd edition, CBS Publication, S.C.Bhatia, 2008.
2. Alla Appa Rao, Engineering Chemistry and Environmental Studies, New Age International Publishers, 1st edition, 2010.
3. Mukhyonov(ed), Chemical Technology Vol. I, MIR Publication, Moscow, 3rd edition, 1979.
4. B.N.Chakrabarthy, Industrial Chemistry, Oxford and LBH Publ., New Delhi, 1984.
5. B.K.Sharma, Industrial Chemistry, Goel Publishing House, 6th edition, 1994.

Part III – Core Lab I – Organic Chemistry Practical I

Hours per week: 4 **Credits: 4**

Subject Code: P1CHC2P1

Qualitative analysis and Organic preparations

Separation and analysis of three component mixtures: Analysis of the components, preparation of solid derivative and submission of physical constant for the components and its solid derivative, identification of the compounds from spectral data.

Organic preparations: About eight single stage preparations of organic compounds illustrating important synthetic methods.

Part III – Core Lab II – Inorganic Chemistry Practical I

Hours per week: 4 **Credits: 4**

Subject Code: P1CHC2P2

Semi-micro qualitative analysis and complexometric titrations

1. **Semi-micro qualitative analysis:** Analysis of mixture containing two familiar and two less familiar cations from the following: W, Pb, Se, Te, Mo, Cu, Bi, Cd, Ce, Th, Zr, V, Cr, Mn, Al, Ni, Co, Zn, Ba, Sr, Li and Mg. (Insoluble and interfering anions may be avoided).
2. **Complexometric titrations:** Estimation of one metal in the presence of another by EDTA

Part III – Core Lab III – Physical Chemistry Practical I

Hours per week: 3 **Credits: 3**

Subject Code: P1CHC2P3

I. Conductometric experiments

(i) Double displacement and acid base titrations

(a) $NH_4Cl \rightarrow NaOH \rightarrow$ Mixture of CH_3COOH and HCl

(b) $NH_4Cl \rightarrow NaOH \rightarrow$ Mixture of NH_4Cl and HCl

(ii) Precipitation titrations

(a) $Na_2CO_3 \rightarrow Pb(NO_3)_2 \rightarrow Na_2CO_3$

(b) $K_2SO_4 \rightarrow BaCl_2 \rightarrow K_2SO_4$

(iii) Determination of cell constant of a conductivity cell, pH and dissociation constant of week acids.

II. Distribution experiments

(i) Distribution of iodine between CCl_4 and H_2O

(a) Determination of partition coefficient

(b) Determination of equilibrium constant of the reaction $KI + I_2 \rightleftharpoons KI_3$

(c) Determination of concentration of given KI solution by distribution method.

(ii) Distribution of benzoic acid between water and benzene

III. Heat of solvation experiments

(a) KNO_3 in water

(b) Benzoic acid in water

(c) Oxalic acid in water

IV. Kinetic study of the reaction between $K_2S_2O_8$ and KI – second order reaction under equimolar concentration.
