



Department of Pure and Applied Chemistry

University of Kota, Kota

M.Sc. I Semester Chemistry

Lecture Plans for Academic Session 2018-19

Paper-1.1: CHEM-511: Inorganic Chemistry

S. No.	Unit wise Broad Topics of the Syllabus	Tentative Lecture(s) Allotted
Unit-I: Structure and Bonding in Main Group Compounds:		
1.	VSEPR theory – basic assumptions	1
2.	VSEPR theory – examples	2-3
3.	Limitations of VSEPR	4
4.	Walsh diagrams (tri-atomic molecules)	5-6
5.	$d\pi - p\pi$ bonds	7
6.	Bent rule and energetic of hybridization	8-10
7.	General trends in acid-base behaviour of binary oxides	11-13
8.	Problem classes	14-15
Unit-II: Metal-Ligand Bonding in Metal Complexes:		
9.	Limitations of crystal field theory	16
10.	Molecular orbital theory	17-18
11.	Octahedral complexes as examples	19-20
12.	tetrahedral complexes as examples	21-22
13.	square planar complexes as examples	23-24
14.	Π - bonding	25
15.	η^2 systems with reference to molecular orbital theory	26
16.	η^3 systems with reference to molecular orbital theory	27
17.	η^5 systems with reference to molecular orbital theory	28
18.	η^6 systems with reference to molecular orbital theory	29
19.	Problem classes	30
Unit-III: Metal-Ligand Equilibria in Solution:		
20.	Stepwise formation and overall formation constants and their interaction	31-32
21.	trends in stepwise constant	33
22.	factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand	34-37
23.	chelate effect and its thermodynamic origin	38
24.	determination of binary formation constants by pH -metry	39-40
25.	determination of binary formation constants by spectrophotometry	41-42
26.	Problem classes	43-45
Unit-IV: Symmetry and Group Theory in Chemistry:		
27.	Symmetry operations and symmetry elements	46
28.	definition of group, subgroup	47
29.	class, order of group	
30.	relation between order of a finite group and its subgroup	48
31.	similarity transformations and classes	49
32.	molecular point groups and their classification	50
33.	Schönflies symbols	51
34.	representations of groups by matrices (representation for the C_n , C_{nv} , C_{nh} , D_{nh} , etc. groups to be worked out explicitly),	52-55
35.	the great orthogonality theorem (without proof) and its importance	56

36.	characters of a representation	57-58
37.	properties of character of representation	
38.	Problem classes	59-60
Unit-V: Applications of Group Theory in Chemistry:		
39.	Introduction of character tables,	61
40.	formation of character tables of C_{2v} & C_{3v} point groups	62-65
41.	relationship between reducible and irreducible representations	66
42.	formation of hybrid orbitals:- σ -bonding in trigonal planar (BF_3), tetrahedral (CH_4), square pyramid (BrF_5)	67
43.	formation of hybrid orbitals: tetrahedral (CH_4), square pyramid (BrF_5)	68-69
44.	formation of hybrid orbitals: square planar [$Pt(Cl_4)^{2-}$, XeF_4]	70-71
45.	symmetry aspects of molecular vibrations of H_2O , NH_3 in IR and Raman spectroscopy	72-73
46.	Problem classes	74-75

Range of lectures required for completion of broad topics of the Syllabus : 65-75

Books:

- *Advanced Inorganic Chemistry*, F.A. Cotton and Wilkinson, John Wiley.
- *Inorganic Chemistry*, J.E. Huhey, Harpes & Row.
- *Chemistry of the Elements*. N.N. Greenwood and A. Earnshaw, Pergamon.
- *Concepts and Models of Inorganic Chemistry*, 3rd edition, B. Douglas, D. McDaniel and J. Alexandar, Wiley.
- *Magneto-chemistry*, R.L. Carlin, Springer Verlag.
- *Comprehensive Coordination Chemistry eds.*, Wilkinson, Gillars and Mc Cleverty, Pergamon.
- *Group Theory*, Patel & Patel
- *Chemical Applications of Group Theory*, F. A. Cotton.
- *Group Theory and its Application*, P. Bhattacharya, Himalaya Publication
- *Group Theory and its Application*, Ramashanker & S. C. Ameta, Sadguru Publication
- *Group Theory and its Application*, Ramakrishanan and Swaminathan, Vishal Publication.

Paper-II: CHEM-512: Organic Chemistry

S. No.	Unit wise Broad Topics of the Syllabus	Tentative Lecture(s) Allotted
Unit-I: Nature of Bonding in Organic Molecules:		
1.	Delocalized chemical bonding: conjugation, cross-conjugation, resonance, hyper-conjugation, bonding in fullerenes, tautomerism;	1-4
2.	Hückel's rule, aromaticity in benzenoid and non-benzenoid compounds	5-7
3.	anti-aromaticity, homo-aromaticity	8
4.	alternant and non-alternant hydrocarbons	9
5.	energy level of π -molecular orbitals, annulenes,	10
6.	bonds weaker than covalent bond: addition compounds (crown ether complexes and cryptands)	11-13
7.	inclusion compounds (catenanes and rotaxanes)	14-15
Unit-II: Structure and Reactivity:		
8.	Thermodynamic and kinetic aspects of reactions	16
9.	resonance and field effects, steric effect, isotope effect, effects of structure on reactivity	17-18
10.	The Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation	19-20
Reaction Mechanism:		
11.	Types of reaction mechanism, potential energy diagram, transition states and intermediates	21
12.	methods of determining mechanisms (product analysis, intermediates analysis,	22-25

	isotope effect, kinetic and stereochemical studies)	
	Reactions Intermediates:	
13.	Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzyne and nitrenes	26-30
Unit-III: Stereochemistry:		
14.	Conformational analysis of cycloalkanes & decalins, conformation of sugars	31-32
15.	effect of conformation on reactivity	33
16.	strain due to unavoidable crowding	34
17.	elements of symmetry, chirality, molecules with more than one chiral centre, threo and erythro isomers	35-36
18.	methods of resolution	37
19.	optical purity, enantiotopic and diastereotopic atoms, groups and faces	38
20.	stereospecific and stereoselective synthesis	39
21.	optical activity in the absence of chiral carbon (biphenyls, allenes and spirane)	40
22.	chirality due to helical shape	41
23.	invertomers	42
24.	asymmetric synthesis	43
25.	determination of configuration (absolute & relative) and conformation	44-45
Unit-IV: Aliphatic Nucleophilic Substitution Reactions:		
26.	The S _N 2, S _N 1, mixed S _N 1 & S _N 2, S _N i and SET mechanisms	46
27.	Aliphatic Nucleophilic Substitution: reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium	47-48
28.	neighbouring group participation by π- and σ-bonds	49
29.	classical and non-classical carbocations, phenonium ions, norbornyl systems	50
30.	rearrangement of epoxides, transannular rearrangement	51
31.	nucleophilic substitution at vinylic, allylic and aliphatic trigonal carbon	52
32.	phase transfer catalysis	53-54
33.	ambient nucleophiles, regioselectivity	55-56
Aromatic Nucleophilic Substitution Reactions:		
34.	S _N Ar S _N 1, S _N Ar S _N 2, benzyne and S _{RN} 1 mechanisms	57
35.	Aromatic Nucleophilic Substitution: reactivity effects of substrate structure, leaving group and attacking nucleophile	58-59
36.	von Richte, Sommelet-Hauser, and Smiles rearrangements	60
Unit-V: Aliphatic Electrophilic Substitution Reactions:		
37.	Bimolecular mechanisms SE2, SE1, SEi mechanism	61
38.	electrophilic substitution accompanied by double bond shifts	
39.	effect of substrates, leaving groups and the solvent polarity on the reactivity	62
Aromatic Electrophilic Substitution Reactions:		
40.	Arenium ion mechanism	63
41.	orientation and reactivity in benzene ring, energy profile diagrams	
42.	ortho/para ratio, ipso attack	64
43.	orientation and reactivity in other ring systems	65
44.	quantitative treatment of reactivity in substrates and electrophiles, diazonium coupling	66
45.	Vilsmeier-Haack reaction, Reimer-Tiemann reaction, Gatterman-Koch reaction, Houben-Hoesch reaction, Fries rearrangement, Bischler-Napieralski reaction	67-75

Range of lectures required for completion of broad topics of the Syllabus : 65-75

Books:

- *Structure and Mechanism in Organic Chemistry*, C.K. Ingold, Cornell University Press.
- *Organic Chemistry*, Clayden, Nick Greeves and Stuart Warren, Oxford University Press

- *Advanced Organic Chemistry: Reactions, Mechanism and Structure*, Jerry March, John Wiley.
- *Advanced Organic Chemistry, Part A and Part B*, F.A. Carey and R.J. Sundberg, Plenum.
- *A Guide Book to Mechanism in Organic Chemistry*, Peter Sykes, Longman.
- *Organic Chemistry*, R. T. Morrison and R. N. Boyd, Prentice-Hall.
- *Reaction Mechanism in Organic Chemistry*, S. M. Mukherjee and S. P. Singh, Macmillan.
- *Textbook of Organic Chemistry* by P S Kalsi, New Age International
- *Organic Reactions, Stereochemistry and Mechanism (Through Solved Problems)* by PS Kalsi, New Age
- *Stereochemistry of Carbon Compounds*, Ernest L. Eliel, TataMcGraw Hill.
- *Stereochemistry of Organic Compounds*, D. Nasipuri, New Age International.
- *Stereochemistry of Organic Compounds*, P.S. Kalsi, New Age International.
- *Stereochemistry, Conformation and Mechanism* by P S Kalsi, New Age International

Paper-III: CHEM-513: Physical Chemistry

S. No.	Unit wise Broad Topics of the Syllabus	Tentative Lecture(s) Allotted
Unit-I: Quantum Chemistry-I:		
1.	Introduction to quantum mechanics and Schrodinger equation	1-2
2.	the postulates of quantum mechanics and numerical	3-4
3.	discussion of solutions of the Schrodinger equation to some model	5-6
4.	Schrodinger equation to harmonic oscillator, rigid rotor, hydrogen atom	7-8
Approximate Methods:		
5.	The variation theorem and its applications	9-10
6.	Linear variation principle,	11
7.	perturbation theory (first order and non-degenerate) and perturbation	12-13
8.	applications of variation method and perturbation theory to Helium atom.	14-15
Unit-II: Quantum Chemistry-II:		
Angular Momentum:		
9.	Ordinary angular momentum,	16
10.	generalized angular momentum,	17
11.	Eigen functions and Eigen values for angular momentum,	18-19
12.	operator using Ladder operators addition of angular momentum	20-21
Molecular Orbital Theory:		
13.	Hückel theory of conjugated systems	22
14.	bond and charge density calculations,	23-25
15.	applications to ethylene, butadiene, cyclopropenyl radical cyclobutadiene,	26-29
16.	introduction to extended Hückel theory.	30
Unit-III: Chemical Dynamics:		
17.	Methods of determining rate laws,	31
18.	collision theory of reaction rates, activated complex theory,	32-33
19.	steric factors,	34
20.	kinetic salt effects, steady state kinetics,	35-36
21.	kinetic and thermodynamic control of reactions	37
22.	Dynamics of chain reactions (hydrogen-bromine reaction),	38
23.	photochemical reactions (hydrogen-bromine and hydrogen-chlorine reactions),	39
24.	kinetics of enzyme catalyzed reactions,	40-41
25.	general features of fast reactions,	42
26.	study of fast reactions (flow method, relaxation method, flash photolysis),	43-44
27.	dynamics of unimolecular reactions (Lindemann Hinshelwood and Rice-Ramsperger-Kassel-Marcus).	45
Unit-IV: Adsorption:		
28.	Surface tension, capillary action,	46

29.	pressure difference across curved surface (Laplace equation),	47-48
30.	vapour pressure of droplets (Kelvin equation),	49
31.	Gibbs adsorption isotherm,	50
32.	estimation of surface area (BET equation),	51
33.	surface films on liquids (Electro-kinetic phenomenon),	52
34.	catalytic activity at surfaces, different isotherms,	53-54
	Micelles:	
35.	Surface active agents, classification of surface active agents,	55
36.	micellization, hydrophobic interaction,	56
37.	critical micellar concentration (CMC), factors affecting the CMC of surfactants,	57
38.	counter ion binding to micelles,	58
39.	thermodynamics of micellization-phase separation and mass action models,	59
40.	solubilisation, micro emulsion, reverse micelles.	60
Unit-V: Macromolecules:		
41.	Definition & types of polymers, mechanism of polymerization,	61-62
42.	electrically conducting, fire resistant, liquid crystal polymers,	
43.	kinetics of polymerization,	63-64
44.	molecular mass determination (osmometry, viscometry, diffusion, light scattering and sedimentation methods),	65-70
45.	chain configuration of macromolecules,	71-72
46.	calculation of average dimension of various chain structures.	73-75

Range of lectures required for completion of broad topics of the Syllabus : 65-75

Books:

- *Physical Chemistry, P.W. Atkins, ELBS.*
- *Introduction to Quantum Chemistry, A.K. Chandra, Tata Mc Graw Hill.*
- *Quantum Chemistry, R. K. Prasad,*
- *Coulson's Valence, R.Mc Weeny, ELBS.*
- *Chemical Kinetics. K.J. Laidler, McGraw-Hill.*
- *Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum.*
- *Modern Electrochemistry Vol. 1 and Vol II J.O.M. Bockris and A.K.N. Reddy, Plenum.*
- *Introduction to Polymer Science, V.R. Gowariker, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.*
- *Advanced Physical Chemistry, Gurudeep Raj, Goel Publication House*
- *Adsorption and Catalysis, G. Whitmore, Sarup & Sons Publishers.*

Paper-IV: CHEM-514: Mathematics for Chemists

(For students without Mathematics in B. Sc.)

S. No.	Unit wise Broad Topics of the Syllabus	Tentative Lecture(s) Allotted
Unit-I: Basic Mathematics:		
1.	Matrix algebra,	1-2
2.	determinants,	3-4
3.	linear equations,	5-6
4.	Eigen values and Eigen vectors,	7-8
5.	basic rules for differentiation,	9-10
6.	partial differentiations,	11-12
7.	maxima and minima,	13-14
8.	basic rules for integration,	15
Unit-II: Mathematics and Linear Programming Problems:		
9.	Basic concepts of differential equations,	16-17
10.	solution of linear differential equations of constant coefficients,	18-20

11.	Vectors: definition dot,	21-22
12.	triple and cross product,	23-24
13.	Vector Calculus: gradient,	25-26
14.	divergence and curl	27-28
15.	linear programming problems: Formulation, graphical solution,	29-30
Unit-III: Basic Operations Research:		
16.	Operations research - concept and applications of OR,	31-33
17.	transportation problem,	34-38
18.	assignment problems,	39-41
19.	basic concepts of inventory control,	42-45
Unit-IV: Basic Statistics:		
20.	Basic concept of statistics	46
21.	representation of data-histogram	47
22.	Pie chart	48
23.	measures of central tendency	49
24.	deviation,	50-51
25.	dispersion,	52-53
26.	skewness and kurtosis,	54-55
27.	random variables, mathematical expectations	56
28.	correlation	57-58
29.	regression	59-60
Unit-V: Statistical Inference:		
30.	Probability theory	61
31.	probability distribution: discrete (binomial and Poisson),	62-63
32.	sampling concepts,	64-65
33.	sampling test for mean	66-67
34.	testing of hypothesis	68-70
35.	test based on t-distribution (t-test)	71-75

Range of lectures required for completion of broad topics of the Syllabus : 65-75

Books:

- *Mathematical Statistics-Gupta and Kapoor.*
- *Operations Research-Kanti Swaroop.*
- *The Chemistry Mathematics Book, E. Steiner, Oxford University Press.*
- *Mathematics for Chemistry, Doggett and Sucliffe, Longman.*
- *Mathematical for Physical Chemistry: F. Daniels, Mc Graw Hill.*
- *Chemical Mathematics D.M. Hirst, Longman.*
- *Applied Mathematics for Physical Chemistry, J.R. Barrnte, Prentice Hall.*
- *Basic Mathematics for Chemists, Tebbutt, Wiley.*

OR

Paper-IV: CHEM-514: Biology for Chemists

(For students without Biology in B. Sc.)

S. No.	Unit wise Broad Topics of the Syllabus	Tentative Lecture(s) Allotted
Unit-I: Cell Structure and Functions:		
1.	Structure of prokaryotic	1
2.	structure of eukaryotic cells,	2-3
3.	intracellular organelles and their functions,	4-6
4.	comparisons of plant and animal cells,	7
5.	overview of metabolic processes: catabolism and anabolism,	8-11
6.	origin of life: unique properties of carbon,	12-13

7.	chemical evolution and rise of living systems.	14-15
Unit-II: Carbohydrates:		
8.	Monosaccharides: Structure, conformation	16-17
9.	functions of important derivatives of monosaccharides;	18-19
10.	structural polysaccharides: cellulose and chitin,	20-22
11.	storage polysaccharides: starch and glycogen,	23-25
12.	structure and biological functions of glucosaminoglycans or mucopolysaccharides,	26-27
13.	glycoproteins and glycolipids,	28-29
14.	role of sugars in biological recognition.	30
Unit-III: Lipids:		
15.	Fatty acids,	31
16.	structure and function of triacylglycerols,	32-33
17.	structure and function of cholesterol, bile acids,	34-36
18.	lipoproteins: composition and function,	37
19.	role in atherosclerosis;	38
20.	properties of lipid aggregates: micelles, bilayers, liposomes	39-40
21.	biological membranes,	41
22.	fluid mosaic model of membrane structure,	42-43
23.	lipid metabolism: β -oxidation of fatty acids.	44-45
Unit-IV: Amino-acids and Proteins:		
24.	Amino acid metabolism: degradation and biosynthesis of amino acids,	46-47
25.	sequence determination: chemical / enzymatic / mass spectral, racemization / detection,	48-50
26.	Chemical and enzymatic hydrolysis of proteins,	51
27.	secondary structure of proteins,	52-53
28.	force responsible for holding of secondary structures,	54
29.	α -helix, β -sheets,	55-56
30.	tertiary structure of protein: folding and domain structure,	57-58
31.	quaternary structure	59-60
Unit-V: Nucleic Acids:		
32.	Purine and pyrimidine bases of nucleic acids,	61
33.	structure of ribonucleic acids (RNA)	62-63
34.	structure of deoxyribonucleic acid (DNA),	64-65
35.	double helix model of DNA,	66-67
36.	chemical and enzymatic hydrolysis of nucleic acids,	68
37.	chemical basis of heredity,	69
38.	an overview of replication,	70-71
39.	transcription,	72-73
40.	translation and genetic code,	74-75

Range of lectures required for completion of broad topics of the Syllabus : 65-75

Books:

- *Principles of Biochemistry*, A.L. Lehninger, Worth Publishers.
- *Biochemistry*, L. Stryer, W.H. Freeman.
- *Biochemistry*, J. David Rawn, Neil Patterson.
- *Biochemistry*, Voet and Voet, John Wiley.
- *Outlines of Biochemistry* E.E. Conn and P.K. Stumpf, John Wiley.



Department of Pure and Applied Chemistry

University of Kota, Kota

M.Sc. II Semester Chemistry

Lecture Plans for Academic Session 2018-19

Paper-2.1: CHEM-521: Inorganic Chemistry

S. No.	Unit wise Broad Topics of the Syllabus	Tentative Lecture(s) Allotted
Unit-I: Reaction Mechanism of Transition Metal Complexes-I:		
1.	Energy profile of a reaction,	1
2.	reactivity of metal complex,	2
3.	inert and labile complexes,	3-4
4.	kinetic application of valence bond and crystal field theories,	5-6
5.	kinetics of octahedral substitution,	7
6.	acid hydrolysis, factors affecting acid hydrolysis,	8-9
7.	base hydrolysis,	10
8.	conjugate base mechanism,	11
9.	direct and indirect evidences in favour of conjugate mechanism,	12
10.	anation reactions,	13-14
11.	reactions without metal ligand bond cleavage	15
Unit-II: Reaction Mechanism of Transition Metal Complexes-II:		
12.	Substitution reactions in square planar complexes,	16-17
13.	the trans effect,	18
14.	mechanism of the substitution reaction,	19
15.	redox reactions,	20-21
16.	electron transfer reactions,	22-23
17.	mechanism of one electron transfer reactions,	24
18.	outer sphere type reactions,	25
19.	inner sphere type reactions	26
20.	cross reactions	27-28
21.	Marcus-Hush theory	29-30
Unit-III: Electromagnetic Spectra and Magnetic Properties of Transition Metal Complexes:		
22.	Spectroscopic ground states,	31
23.	correlation (d^2 and d^3 in octahedral and tetrahedral symmetry),	32-33
24.	Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1 - d^5 states),	34-35
25.	calculations of Dq , B and β parameters using simplified T-S diagrams,	36-37
26.	charge transfer spectra,	38
27.	introduction about circular dichroism	39
28.	introduction about optical rotatory dispersion,	40
29.	spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information,	41-42
30.	anomalous magnetic moments,	43
31.	magnetic exchange coupling and spin crossover	44-45
Unit-IV: Metal π-Complexes:		
32.	Metal carbonyls of Fe, Co & Ni,	46-48
33.	structure and bonding,	49

34.	vibrational spectra of metal carbonyls for bonding and structural elucidation,	50-51
35.	important reactions of metal carbonyls	52-53
36.	preparation, bonding structure and important reaction of transition metal nitrosyls,	54-55
37.	dinitrogen complexes	56-57
38.	dioxgen complexes	58-59
39.	tertiary phosphine as ligand	60
Unit-V: Metal Clusters:		
40.	Higher boranes: Wade's rule, styx numbers & structures,	61-63
41.	carboranes,	64-66
42.	metalloboranes,	67-68
43.	metallocarboranes,	69-70
44.	metal carbonyl and halide clusters,	71-73
45.	compounds with metal-metal multiple bonds.	74-75

Range of lectures required for completion of broad topics of the Syllabus : 65-75

Books:

- *Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.*
- *Inorganic Chemistry, J.E. Huhey, Harpes & Row.*
- *Chemistry of the Elements. N.N. Greenwood and A. Earnshaw, Pergamon.*
- *Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.*
- *Magneto-chemistry, R.L. Carlin, Springer Verlag.*
- *Comprehensive Coordination Chemistry eds., Wilkinson, Gillars and Mc Cleverty, Pergamon.*

Paper-2.2: CHEM-522: Organic Chemistry

S. No.	Unit wise Broad Topics of the Syllabus	Tentative Lecture(s) Allotted
Unit-I: Free Radical Reactions :		
1.	Types of free radical reactions,	1
2.	free radical substitution mechanisms,	
3.	neighbouring group assistance,	2-3
4.	reactivity for aliphatic and aromatic substrates at a bridgehead carbon,	4
5.	reactivity in the attacking radicals,	5
6.	effect of solvents on reactivity,	6
7.	allylic halogenation (NBS),	7
8.	oxidation of aldehydes to carboxylic acids,	8
9.	auto-oxidation,	9
10.	coupling of alkynes and arylation of aromatic compounds by diazonium salts,	10
11.	Sandmeyer reaction, Hunsdiecker reaction, free radical rearrangements.	11
Elimination Reactions:		
12.	E2, E1 and E1cB mechanisms and their spectrum,	12
13.	orientation of the double bond,	13
14.	reactivity effects of substrate str., attacking base, leaving group and medium;	14
15.	mechanism and orientation in pyrolytic elimination	15
Unit-II: Addition to Carbon-Carbon Multiple Bonds :		
16.	Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals	16
17.	regio-and chemoselectivity	17
18.	orientation and reactivity	18
19.	addition to cyclopropane ring	19
20.	hydrogenation of double and triple bonds,	20

21.	hydrogenation of aromatic rings,	
22.	hydroboration,	21
23.	hydroxylation,	
24.	Michael reaction,	22
25.	Sharpless asymmetric epoxidation	
	Addition to Carbon-Hetero Multiple bonds:	
26.	Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles;	23
27.	addition of Grignard reagents, organozinc and organolithium reagents to carbonyl group and unsaturated carbonyl compounds,	24
28.	mechanism of condensation reactions: Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin, Stobbe, Dieckmann reactions, Robinson annulations, Reformatsky reaction, Wittig reaction,	25-29
29.	hydrolysis of esters and amides,	30
30.	ammonolysis of esters	
	Unit-III: Photochemistry-I:	
31.	Photochemical reactions, basic principles,	31
32.	types of excitations,	32
33.	energy dissipation, fate of excited molecule,	33
34.	energy transfer,	34
35.	quantum yield,	35
36.	actinometry;	
37.	photochemistry of alkenes: inter- & intra-molecular reactions of the olefinic bond, addition reactions, cis-trans isomerisation, photo-oxidation reactions, cyclisation reactions,	36-40
38.	photochemistry of 1,3-, 1,4- and 1,5-dienes; photochemistry of aromatic compounds: excited states of benzene, isomerisations, dimerisation, additions and substitutions, photo-reduction, photo-Fries rearrangement;	41-44
39.	photochemistry of vision	45
	Unit-IV: Photochemistry-II:	
40.	Photochemistry of carbonyl compounds: photochemical reactions of cyclic and acyclic saturated carbonyl compounds; bond cleavage, photo-reduction,	46-49
41.	cyclo-addition reactions: dimerisations and oxetane formation;	50-52
42.	photochemical reactions of α,β -unsaturated carbonyl compounds: hydrogen abstraction reactions, photo-cycloadditions, photodimerization,	53-55
43.	rearrangements: cyclohexenones and cyclohexadienones;	56-57
44.	photochemical reactions of β,γ -unsaturated carbonyl compounds: cleavages, rearrangements	58-60
	Unit-V: Pericyclic Reactions:	
45.	Molecular orbitals and their symmetry, m -plane and C_2 -axis,	61
46.	frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system;	
47.	classification of pericyclic reactions,	62
48.	analysis of reactions: Woodward-Hoffmann correlation diagrams, FMO and PMO approach;	63-64
49.	electrocyclic reactions: conrotatory and disrotatory motions, $4n$, $4n+2$ and allyl systems;	65-66
50.	cycloaddition reactions: antarafacial and suprafacial additions,	67
51.	$4n$ and $4n+2$ systems, $2+2$ addition of ketenes, 1,3-dipolar cycloadditions and cheletropic reactions;	68-70
52.	sigmatropic rearrangements: suprafacial and antarafacial shifts of H atom and	71-72

	carbon moieties,	
53.	3,3- and 5,5 sigmatropic rearrangements,	73
54.	Claisen, Cope and aza-Cope rearrangements;	74
55.	Ene reaction	75

Range of lectures required for completion of broad topics of the Syllabus : 65-75

Books:

- *Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.*
- *Organic Chemistry, Clayden, Nick Greeves and Stuart Warren, Oxford University Press*
- *Advanced Organic Chemistry: Reactions, Mechanism and Structure, Jerry March, John Wiley.*
- *Advanced Organic Chemistry, Part A and Part B, F.A. Carey and R.J. Sundberg, Plenum.*
- *A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.*
- *Organic Chemistry, R. T. Morrison and R. N. Hall, Prentice-Hall.*
- *Reaction Mechanism in Organic Chemistry, S. M. Mukherjee and S. P. Singh, Macmillan.*
- *Textbook of Organic Chemistry by P S Kalsi, New Age International*
- *Organic Reactions, Stereochemistry and Mechanism (Through Solved Problems) by P S Kalsi*
- *Stereochemistry of Carbon Compounds, Ernest L. Eliel, TataMcGraw Hill.*
- *Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.*
- *Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.*
- *Pericyclic Reactions, S.M. Mukherjee, McMillan, India.*

Paper-2.3: CHEM-523: Physical Chemistry

S. No.	Unit wise Broad Topics of the Syllabus	Tentative Lecture(s) Allotted
Unit-I: Classical Thermodynamics:		
1.	Brief resume of concepts of laws of thermodynamics,	1
2.	free energy, chemical potential and entropies,	
3.	partial molar free energy, partial molar volume and partial molar heat content and their significance, determinations of these quantities,	2-7
4.	concept of fugacity and determination of fugacity	8-9
Non-ideal Systems:		
5.	Activity, activity coefficient,	10
6.	Debye-Hückel theory for activity coefficient of electrolytic solutions,	11-13
7.	determination of activity and activity coefficients,	14
8.	ionic strength	15
Unit-II: Statistical Thermodynamics :		
9.	Concept of distribution,	16
10.	thermodynamic probability and most probable distribution,	
11.	ensemble averaging, postulates of ensemble averaging,	17-18
12.	canonical, grand canonical and micro-canonical ensembles,	19-20
13.	corresponding distribution laws (using Lagrange's method of undetermined multipliers),	21-22
14.	partition functions-translation, rotational, vibrational and electronic partition functions, and calculation of thermodynamic properties in terms of partition,	23-24
15.	application of partition functions	25
Heat Capacity Behaviour of Solids:		
16.	Chemical equilibria, equilibrium constant,	26
17.	Fermi-Dirac statistics,	27
18.	distribution law, applications to metals and helium,	28-29
19.	Bose-Einstein statistics	30
Unit-III: Non-equilibrium Thermodynamics:		
20.	Thermodynamic criteria for non-equilibrium states,	31

21.	entropy production and entropy flow,	32-33
22.	entropy balance equations for different irreversible processes (<i>e.g.</i> heat flow, chemical reaction, <i>etc.</i>)	34-36
23.	transformations of the generalized fluxes and forces,	37
24.	non-equilibrium stationary states,	38
25.	phenomenological equations,	39
26.	microscopic reversibility and Onsager's reciprocity relations,	40-42
27.	diffusion, electric conduction,	43-44
28.	irreversible thermodynamics for biological systems	45
Unit-IV: Electrochemistry:		
29.	Debye-Huckel-Onsager treatment and its extension,	46
30.	Ion-solvent interactions,	47
31.	Debye-Hückel-Jerum mode,	48
32.	thermodynamics of electrified interface equations,	49
33.	derivation of electro-capillarity,	50
34.	Lippmann equations (surface excess), methods of determination,	51-52
35.	structure of electrified interfaces,	53
36.	Guoy-Chapman, Stern, Bockris, Devanathan models,	54-55
37.	over potentials,	56
38.	exchange current density,	57
39.	derivation of Butler-Volmer equation,	58-59
40.	Tafel plot	60
Unit-V: Electrical Double Layer at Metal/Semiconductor-Electrolyte Interface:		
41.	Thermodynamics of double layer,	61
42.	determination of surface excess charge and other electrical parameters-electrocapillarity, excess charge capacitance, and relative surface excesses,	62-65
43.	metal/ water interaction-contact adsorption, its influence on capacity of interface,	66-67
44.	complete capacity-potential curve, constant capacity region hump,	68-69
45.	semiconductor/electrolyte interface,	70
46.	capacity of space- charge,	71
47.	Mott-Schottky plot	
Polarography:		
48.	Theory, Ilkovic equation,	72
49.	half wave potential and its significance,	73
50.	introduction to corrosion, homogenous theory, forms of corrosion monitoring and prevention methods	74-75

Range of lectures required for completion of broad topics of the Syllabus : 65-75

Books:

- *Physical Chemistry, P.W. Atkins, ELBS.*
- *Introduction to Quantum Chemistry, A.K. Chandra, Tata Mc Graw Hill.*
- *Quantum Chemistry, Ira N. Levine, Prentice Hall.*
- *Coulson's Valence, R.Mc Weeny, ELBS.*
- *Chemical Kinetics. K.J. Laidler, McGraw-Hill.*
- *Kinetics and Mechanism of Chemical Transformation J.Rajaraman and J. Kuriacose, Mc Millan.*
- *Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum.*
- *Modern Electrochemistry Vol. I and Vol II J.O.M. Bockris and A.K.N. Reddy, Planum.*
- *Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern*

Paper-2.4: CHEM-524: Computer Applications in Chemistry

S. No.	Unit wise Broad Topics of the Syllabus	Tentative Lecture(s) Allotted
Unit-I: General Introduction:		
1.	Elements of a computer system,	1
2.	block diagram of computer system and function of its components,	2-3
3.	concept of hardware and software,	4-5
4.	memory,	6
5.	introduction to operating systems (DOS, Windows)	7-8
PC Software:		
6.	Word processing: Creating and saving documents,	9
7.	formatting,	10
8.	inserting tables and pictures,	11
9.	mail merge,	12
10.	spread sheets, charts, graphs and use of functions,	13-14
11.	introduction to presentation packages, graphics and animation	15
Unit-II: Report Generation and Presentation:		
12.	MS Office: Introduction to Word, Excel and Power Point;	16-17
13.	MS Word: Documentation and manipulation, saving and printing, incorporation of graphs, tables pictures and chemical structures into the documents;	18-22
14.	MS Excel: Spread sheets, report generation, cell manipulation, data based management, graphical representation of tabulated data, Pi-chart, bar and line graphs, surface and 3D graphs;	23-27
15.	Power Point: Application of power point for the presentation of reports and slides	28-30
Unit-III: Computing and Languages:		
16.	Elements of programming languages,	31-32
17.	constants and variables,	33-34
18.	operations	35
19.	symbol expressions,	36
20.	flow chart, functions and subroutines,	37-39
21.	graphics, statements,	40
22.	commands,	41
23.	commands for accessing hardware,	42
24.	elements of C language.	43-44
25.	Windows: Introduction and applications.	45
Unit-IV: Computer Applications in Chemistry:		
26.	Introduction to CAD: A balance approach to computer aided process design,	46-49
27.	computer interface with instruments and laboratory information system	49-53
28.	computers in fault & true analysis,	54-56
29.	computers in communication	57-58
30.	Internet: basic concepts, importance in chemical industries	59-60
Unit-V: Computation in Chemistry:		
31.	Computation in chemistry such as pressure from Van der Waals equation,	61
32.	pH of solution,	62
33.	kinetics,	63
34.	radioactive decay,	64
35.	lattice energy,	65
36.	determination of order of reaction,	66

37.	Pauling's relation,	67
38.	ionic radii,	68
39.	molecular weight of an organic compound,	69
40.	resonance energy,	70
41.	isoelectric point of amino acids,	71
42.	Lambert-Beer's law,	72
43.	bond lengths,	73
44.	bond angles,	74
45.	linear simultaneous equations to solve secular equations within the Hückel theory	75

Range of lectures required for completion of broad topics of the Syllabus : 65-75

Books:

- *The Big Basic Book of Window 98: Kraynak-PHI.*
- *Computational Chemistry: A.C. Norris.*
- *Programming in basic problems solving with the true and style: Stewart M. Venit Jaico.*
- *Mastering Windows Special edition: Robert Cowart - BPB Publications.*
- *Computer Fundamental Architecture Organisation: B. Ram - New Age international.*
- *Computers in Chemistry: K.V. Raman - TMH Pub.*
- *Fundamentals of Computer : V. Rajaraman (Prentice Hall)*
- *Computers in Chemistry : K.V. Raman (Tata Mc Graw Hill)*
- *Computer Programming in FORTRAN IV-V Rajaraman (Prentice Hall)*

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