Department of Chemistry (PG)
(2017 Onwards)

M.Sc. Chemistry Course structure (CBCS)

	Course	H/W	C		Course	H/W	C
I Semester	Core 1 (C1)	6	5	**II Semester**	Core 4 (C4)	6	5
	Core 2 (C2)	6	5		Core 5 (C5)	6	5
	Core 3 (C3)	6	5		Core 6 (C6)	6	5
	Core Elective – 1 (A/B) (CE1A/CE1B)	4	3		Core Elective – 2 (A/B) (CE2A/CE2B)	4	3
	Core Practical – I* (CP1)	4	-		Core Practical – I* (CP1)	4	3
	Core practical – II* (CP2)	4	-		Core practical – II* (CP2)	4	3
	Core Practical – III* (CP3)	4	-		Core Practical – III* (CP3)	4	3
					Elective Practical –I	4	
	Total	30	18		Total	30	27

	Course	H/W	C		Course	H/W	C
III Semester	Core 7 (C7)	6	5	**IV Semester**	Core 10 (C10)	6	5
	Core 8 (C8)	6	5		Core 11(C11)	6	5
	Core 9 (C9)	6	5		Project (P)	8	6
	Core Elective – 3 (A/B)	4	5		Core Elective – 3 (A/B) (CE4A/ CE4B)	3	3
	Core Practical – IV* (CP4)	3	-		Core Practical – IV* (CP4)	3	2
	Core practical – V* (CP5)	3	-		Core practical – V* (CP5)	3	2
	Core Practical – VI* (CP6)	3	-		Core Practical – VI* (CP6)	3	2
					Elective Practical –II	4	
	Total	30	20		Total	30	25

* Practical Examinations will be conducted at the end of Even Semester

Distribution of Hours, Credits, No. of Papers, & Marks

Subject	Hours	Credits	No of papers	Marks
Core + Practical	105	76	12+6	1800
Elective (Major) + Practical	12	9	4+2	300
Total	**120**	**90**	**24**	**2200**

Total Credit = 90 credits
Total Hrs / week = 120 Hrs
Papers (22 X 100 marks) = 2200 Marks

Department of Chemistry (PG)								
CBCS Syllabus – M.Sc., Chemistry (2017 onwards)								
Sem	**P**	**Title of the Paper**	**Sub. Code**	**H/ W**	**C**	**Marks**		
						I	**E**	**T**
I	C1	INORGANIC CHEMISTRY – I	15PCHC11	5	5	25	75	100
	C2	ORGANIC CHEMISTRY – I	15PCHC12	5	5	25	75	100
	C3	PHYSICAL CHEMISTRY – I	15PCHC13	5	5	25	75	100
	CE1A	CHROMATOGRAPHY	15PCHE1A	3	3	25	75	100
	CE1B	BIOCHEMISTRY	15PCHE1B					
	CP1	INORGANIC CHEMISTRY PRACTICAL -I	15PCHC2P1	4	--	Exam – II Sem		
	CP2	ORGANIC CHEMISTRY PRACTICAL – I	15PCHC2P2	4	--	Exam – II Sem		
	CP3	PHYSICAL CHEMISTRY PRACTICAL – I	15PCHC2P3	4	--	Exam – II Sem		
II	C4	INORGANIC CHEMISTRY - II	15PCHC21	5	5	25	75	100
	C5	ORGANIC CHEMISTRY – II	15PCHC22	5	5	25	75	100
	C6	PHYSICAL CHEMISTRY – II	15PCHC23	5	5	25	75	100
	CE2A	INSTRUMENTAL METHODS OF ANALYSIS	15PCHE2A	3	3	25	75	100
	CE2B	ENZYME CHEMISTRY	15PCHE2B					
	CP1	INORGANIC CHEMISTRY PRACTICAL -I	15PCHC2P1	4	3	40	60	100
	CP2	ORGANIC CHEMISTRY PRACTICAL – I	15PCHC2P2	4	3	40	60	100
	CP3	PHYSICAL CHEMISTRY PRACTICAL -I	15PCHEC2P 3	4	3	40	60	100
III	C7	INORGANIC CHEMISTRY - III	15PCHC31	5	5	25	75	100
	C8	ORGANIC CHEMISTRY – III	15PCHC32	5	5	25	75	100
	C9	PHYSICAL CHEMISTRY – III	15PCHC33	5	5	25	75	100
	NME	CHEMINFORMATICS (OR) APPLIED CHEMISTRY	15PCHN31A 15PCHN31B	6	5	25	75	100
	CE3B	----------						
	CP4	INORGANIC CHEMISTRY PRACTICAL-II	15PCHC4P1	3	--	Exam – IV Sem		
	CP5	ORGANIC CHEMISTRYPRACTICAL – II	15PCHC4P2	3		Exam – IV Sem		
	CP6	PHYSICAL CHEMISTRY PRACTICAL-II	15PCHC4P3	3	--	Exam – IV Sem		
IV	C8	ORGANIC CHEMISTRY – IV	15PCHC41	5	5	25	75	100
	C9	PHYSICAL CHEMISTRY – IV	15PCHC42	5	5	25	75	100
	P	PROJECT	15PCHP41	8	6	0	100	100
	CE4A	MEDICINAL CHEMISTRY	15PCHE4A	3	3	25	75	100
	CE4B	RATIONAL DRUG DESIGN	15PCHE4B					
	CP4	INORGANIC CHEMISTRY PRACTICAL	15PCHC4P1	3	2	40	60	100
	CP5	ORGANIC CHEMISTRY PRACTICAL - II	15PCHC4P2	3	2	40	60	100
	CP6	PHYSICAL CHEMISTRY PRACTICAL	15PCHC4P3	3	2	40	60	100
Total				**120**	**90**	**615**	**1585**	**2200**

DEPARTMENT OF CHEMISTRY (PG)

Non-Major Elective Course offered to Other Major PG Students

SEM	P	Title of the paper	S. Code	H/W	C	Marks		
						I	E	T
I	NME	CHEMINFORMATICS (OR) APPLIED CHEMISTRY	15PCHN31A (OR) 15PCHN31B	6	5	25	75	100

LIST OF NON-MAJOR ELECTIVE COURSES OFFERED TO PG STUDENTS BY VARIOUS DEPARTMENTS

SEM	TITLE OF THE PAPER	S.CODE	H/W	C	MARKS		
					I	E	T
DEPT. OF ENGLISH (PG)							
III	English For Business Communication	15PENN31	6	5	25	75	100
DEPT. OF COMPUTER SCIENCE (PG)							
III	Internet Concepts and Web Design	15PCSN31	6	5	25	75	100
DEPT. OF MATHEMATICS (PG)							
III	Basics in Mathematics	15PMAN31	6	5	25	75	100
DEPT. OF PHYSICS (PG)							
III	Renewable Energy Sources	15PPHN31	6	5	25	75	100
DEPT. OF CHEMISTRY (PG)							
III	Cheminformatics (OR)	15PCHN31A	6	5	25	75	100
	Applied Chemistry	15PCHN31B					
DEPT. OF ZOOLOGY (PG)							
III	Wild life management (OR)	15PZON31A	6	5	25	75	100
	Apiculture	15PZON31B					

Added-striked out, Deleted- highlighted

I SEMESTER			
C1	INORGANIC CHEMISTRY – I		15PCHC11
Hrs / Week: 5	Hrs / Sem.: 75	Hrs / Unit: 15	Credit: 5

UNIT I: SOLID STATE CHEMISTRY

Objective: *To study about crystals and their structural aspects*

Description of crystal structure – Rock salt, Zinc blende, Wurtzite, Fluorite, Antifluorite, Perovskite, $CdCl_2$, Spinel and Rutile. ~~(CsCl, K2NiF, Inverse spinel)~~ Crystal defects – line and plane defects – intrinsic point defects – Schottky and Frenkel defects – Extrinsic point defects – non-stoichiometric defects. Color centres. Electronic structure of solids – Free electron and Band theory.

~~**UNIT II: CHEMICAL BONDING & STEREOCHEMISTRY**~~

~~**Chemical Bonding, Inorganic chains, rings and cages**~~

Objective: *To study the nature of chemical bonding and stereochemistry*

VSEPR theory – concept of hybridization & structure of molecules ~~Postulates and applications of VSEPR theory~~ – Bent's rule – Apicophilicity dπ-pπ bonds, M.O theory – symmetry and overlap – M.O diagram of HF and BeH_2. Walsh diagram (triatomic molecules, ~~BeH2 and CO2~~).

Geometrical isomerism in complexes of coordination numbers 4 & 6 with examples. Different types of electrostatic interactions and their effects on properties Fluxionality – Inversion of pyramidal molecule. Planar – tetrahedral interconversion. Trigonal bipyramidal – square pyramidal interconversion.

~~Chains catenation – heterocatenation Intercalation chemistry – One-dimensional conductors – $(SN)_x$~~

~~Rings – Preparation, properties and Structure of borazine, phosphazene.~~

~~Cages – Preparation and structure of phosphorous cage molecules, Diboranes, tetraboranes. Structures of B_5H_9, B_5H_{11} ,B_6H_{10},~~ $[B_8H_8]^{2-}$, $[B_{12}H_{12}]^{2-}$. ~~Structural relationships of closo, nido and arachno boranes. – Styx number – Carboranes Structure of nido-CB_5H_9, nido-2,3-$C_2B_4H_8$, closo- 1,5-$C_2B_3H_5$ and closo-2,4-$C_2B_5H_7$.~~

UNIT III: **INORGANIC CHAINS, RINGS, AND CAGES.**

~~**STEREOCHEMISTRY & COORDINATION CHEMISTRY-I**~~

Objective*: To know about Inorganic chains, rings and cages.*

Chains catenation – heterocatenation- Intercalation chemistry – One-dimensional conductors – $(SN)_x$

Rings – Preparation, properties and Structure of borazine, phosphazene.

Cages – Preparation and structure of phosphorous cage molecules, Diboranes, tetraboranes. Structures of B_5H_9, B_5H_{11} ,B_6H_{10}, $[B_8H_8]^{2-}$, $[B_{12}H_{12}]^{2-}$. Structural relationships of closo, nido and arachno boranes. – Styx number – Carboranes- Structure of nido-CB_5H_9, nido-2,3-$C_2B_4H_8$, closo- 1,5-$C_2B_3H_5$ and closo-2,4-$C_2B_5H_7$.

~~Geometrical isomerism in complexes of coordination numbers 4 & 6 with examples. Different types of electrostatic interactions and their effects on properties Fluxionality~~

~~IUPAC Nomenclature Structure and isomerism of the following: Coordination number 1, 2, 3, 4 (tetrahedral, square planar), 5 (Trigonal bipyramidal, Square pyramidal), 6, 7 and 8. Optical, Geometrical isomerism in octahedral complexes – Linkage isomerism.~~

UNIT IV: METAL CARBONYLS & METAL CLUSTERS.

~~COORDINATION CHEMISTRY II~~

Objective: *To study about metal carbonyl and metal clusters*

Metal carbonyls – Classification – general methods of preparation, physical and chemical properties, EAN rule, Structure and bonding of metal carbonyls: $Ni(CO)_4$, $Fe(CO)_5$, $Cr(CO)_6$, $Mn_2(CO)_{10}$, $Co_2(CO)_8$, $Fe_2(CO)_9$ – Distinction of bridged and terminal carbonyl using IR spectra Metal nitrosyls – Structure of $[Ir(PPh_3)_2CO(NO)Cl]^+$ and $[Ru(PPh_3)_2(NO)_2Cl]^+$

Metal clusters – Structure of carbonyl clusters – $Ru_3(CO)_{12}$,$Co_4(CO)_{12}$, $Ir_4(CO)_{12}$, $Rh_6(CO)_{16}$, $Ru_6(CO)_{18}H_2$, $[Ni_3(CO)_6]n_2$-, $Fe_5(CO)_{15}C$, $Ru_6(CO)_{17}C$, $[Ru_6N(CO)_{16}]$- Wade's rules – Structure of non carbonyl clusters – $[Re_2X_8]^{2-}$, $Re_2(RCOO)_4X_2$, Re_3Cl_9, $[Mo_6Cl_8]^{4+}$ and $[PbI_5]^{2-}$

~~Crystal Field theory (CFT) Important features – Crystal field Splitting of d- orbitals in octahedral, tetragonal, square planar and tetrahedral complexes – Crystal field splitting energy (CFSE) values – factors affecting the value of Δ. Application of crystal field theory in colour, spectral and magnetic properties – Jahn Teller Effect distortion.~~

UNIT V: NOBLE GASES, PSEUDOHALOGENS & INTERHALOGEN COMPOUNDS

~~COORDINATION CHEMISTRY III~~

Objective: *To study about structure and properties of noble gases, pseudohalogens and interhalogens*

Noble Gas chemistry – Preparation and bonding of Xenon fluorides - Clathrates.

Halogens : Iodine – Basic properties – evidences.

Interhalogen compounds -Preparation, properties, structure and uses of ICl, IBr, BrF_3, ICl_3, ClF_3, IF_5, IF_7.

Polyhalide ions and polyhalides – classification – preparation-properties. Structure and shape of ICl_2^-, ICl_2^+, ICl_4^-, IF_4^+ and higher polyhalide ions, Halogen oxides and oxyfluorides.

Pseudohalogens – Structure, preparation, properties and uses of $(CN)_2$, $(SCN)_2$, $(SeCN)_2$, $(OCN)_2$. Similarities and dissimilarities between halogens and pseudohalogens, halides and pseudohalogens.

~~Molecular Orbital Approach – σ and π bonding in octahedral, tetrahedral and square planar complexes.~~

~~Electronic and steric effect of complexes, Symbiosis. Thermodynamic stability – stepwise stability constant and overall stability constant – log β value and stability. Factors affecting the stability of complexes in solution – Determination of stability constant by Bjerrum method, spectrometric method and Job's method – comparison of thermodynamic and kinetic stability~~

REFERENCE:

1. Solid State Chemistry and its Applications, A.R. West, Wiley, 1984.
2. Solid State Chemistry, N.B. Hannay, Printice-Hall, 1967.
3. Solid State Chemistry D. K. Chakrabarty, New Age International, 2010.
4. Inorganic Chemistry - Principles, structure and reactivity, J E Huheey, Harper and Row Publisher, Inc. New York (1972)
5. Concise Inorganic Chemistry, J. D. Lee, Elbs with Chapman and Hall, London
6. Advanced Inorganic chemistry, F. A. Cotton, R. G. Wilkinson, 6th Edn., Wiley, 1996
7. Modern Inorganic Chemistry, Willam L. Jooly, Magraw-Hill, 1991.
8. Inorganic Chemistry, D.F.Shriver and P.W. Atkins, 4th Edn., Harper Collins, 1993.
9. Modern Inorganic Chemistry, R. D. Madan & Satya Prakash, S Chand and Company, Ltd., 1st Edn., 1987.
10. Inorganic Chemistry, Gary L. Miessle and Donald A. Tarr, Dorling Kindersley (India) Pvt. Ltd., 3rd Edn., 2009.
11. Inorganic Chemistry - Principles, structure and reactivity, IV edition, James E. Huheey, Ellen A Keitier, Richard L Keiter Pearson Publication (2012).

I SEMESTER			
C2	**ORGANIC CHEMISTRY – I**		**15PCHC12**
Hrs / Week: 5	**Hrs / Sem.: 75**	**Hrs / Unit: 15**	**Credit: 5**

UNIT I: REACTIVE INTERMEDIATES, YLIDES AND ENAMINES:

Objective: *To understand the concept of reaction intermediates*

Reaction intermediates:

Carbocation: Structure, formation, stability, evidences, reactions – rearrangements-carbo-cations in annulene, Neighbouring group participation by σ and π bonds. ~~Non classical Carbocations:~~

Neighbouring group participation (C-C, C=C, Cyclopropyl, Aromatic rings as neighbouring group).

Carbanion- Structure, formation, reaction and stability, effect of substituents on resonance stabilized carbanions.

Benzyne- structure, mechanism, evidence and trapping.

Free radicals – Formation, reactions, Stability, Structure.

Carbenes: Structure, generation, Types of carbenes, formation, reactions, stability – addition, insertion reactions, rearrangement reactions.

Arynes- Formation, Reactions, Stability, Structure, trapping

Nitrene, Structure-generation, reaction, insertion, abstraction, rearrangement, addition

Enamines: Generation and reactions, Metalloenamines.

Ylides – Generation and reactions.

Free radicals – stability, generation, reactions.

UNIT II: APPLICATION OF REAGENTS IN OXIDATION and REDUCTION IN ORGANIC SYNTHESIS:

Objective: *To study the oxidation and reduction of compounds and their synthetic applications.*

Oxidation: Application of $KMnO_4$, $K_2Cr_2O_7$, Ozone, Hydrogen peroxide, *t*-butylhydroperoxide, Aluminium *tert*-butoxide, Lead tetraacetate, Periodic acid, N-Bromosuccinimide, Ruthenium tetroxide.

Reduction: Application of Platinum, Palladium, Nickel, Lithium borohydride, Sodium borohydride, Sodium cyanoborohydride – Sodium –amalgam, Sodium –liquid Ammonia, Zinc –Hydrochloric acid, Formic acid, Hydrazine hydrate, Tin-Hydrochloric acid (Sn/HCl), Zinc in Acetic acid (Zn/CH_3COOH), Sodium dithionate.

UNIT III: IMPORTANT REAGENTS IN ORGANIC SYNTHESIS

Objective: *To study the use of various reagents in organic synthesis*

Use of following reagents in Organic Synthesis and functional group transformations: Lithium diisopropylamide (LDA), N,N'-Dicyclohexylcarbodiimide (DCC), Trimethylsilyl iodide, tri-*n*-Butyltin hydride, Osmium tetraoxide, Selenium dioxide, 1,3-Dithianes, 2,3-Dichloro-5,6-Dicyanobenzoquinone (DDQ), Lead tetra acetate, Grignard Reagent.

UNIT IV: SOME NAME REACTIONS IN ORGANIC CHEMISTRY:

Objective: *To study Mechanism of reactions in Organic Chemistry*

Mechanism and their applications in organic synthesis - Aldol condensation, Arndt – Eistert synthesis, Benzoin condensation, Cannizaro reaction, Mannich reaction, Reformatsky reaction, Reimer-Teimann reaction, Biginelli Reaction, Clemmensen reduction, Kolbe-Schmitt Reaction, Schotten-Baumann Reaction, Friedel-Crafts Acylation, Friedel-Crafts Alkylation, Bayer Villiger Oxidation - Swern Oxidation (DMSO/ Dichloromethane).

Coupling Reactions:

Heck reaction, Sonogashira coupling, Suzuki reaction

~~ALIPHATIC NUCLEOPHILIC SUBSTITUTION AND ELIMINATION REACTIONS~~

~~a) Aliphatic Nucleophilic substitutions~~

~~S_N1 and S_N2 mechanisms – effect of substrate, structure, base solvent, the leaving group and the solvent on nucleophilic substitution – Symphoria – Neighboring Group Participation due to σ and π electrons S_N2', S_N1' and S_Ni reactions mechanism.~~

~~b) Elimination Reactions:~~

~~E1, E2 and E1cB mechanisms. Reactivity: effects of substrate structures, attacking base, the leaving group, the nature of medium on elimination reactions – Hofmann, Saytzeff and Bredt's rules. Pyrolytic elimination reactions.~~

~~c) Mechanism of Addition to carbon – carbon double bonds:~~

~~Mechanism and stereochemical aspects hydrogenation, hydrohalogenation – hydroboration – hydroxylation.~~

UNIT V: ALIPHATIC NUCLEOPHILIC SUBSTITUTION AND ELIMINATION REACTIONS

Objective: *To study about the mechanisms in Organic reaction*

a) Aliphatic Nucleophilic substitutions

S_N1 and S_N2 mechanisms – effect of substrate, structure, base solvent, the leaving group and the solvent on nucleophilic substitution – Symphoria – Neighboring Group Participation due to σ and π electrons S_N2, S_N1 and S_Ni reactions mechanism.

b) Elimination Reactions:

E1, E2 and E1cB mechanisms. Reactivity: effects of substrate structures, attacking base, the leaving group, the nature of medium on elimination reactions – Hofmann, Saytzeff and Bredt's rules. Pyrolytic elimination reactions.

c) Mechanism of Addition to carbon – carbon double bonds:

Mechanism and stereochemical aspects hydrogenation, hydrohalogenation – hydroboration – hydroxylation.

~~AROMATICITY, NOVEL RINGS~~

~~a Aromaticity:~~ ~~Huckel's rule- Five, Six, Seven and Eight membered rings, Other systems containing aromatic sextet, Systems of two, four, six, eight, ten and more than ten electrons, Homoaromatic compounds, Fullerenes.~~

~~b. Novel rings:~~ ~~Nomenclature of bicyclic system- Adamantane and tricyclic systems- Cubane.~~

~~c~~~~. Molecular machines-Catenanes, Rotaxanes- Cucurbit[n]uril-Based Gyroscane structure.~~

REFERENCES

1. Advanced Organic Chemistry, Part A: Structure and Mechanisms, F.A. Carey, R.A. Sundberg, 5thEdn., Springer, 2007.

2. Organic Reaction Mechanisms, A.C. Knipe, John Wiley& Sons Ltd. Publications, 2012.
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4. Synthetic Approaches in Organic Chemistry, Raj K. Bansal, Jones and Barlett Publishers, International, 1998.
5. Advanced Organic Chemistry: Reaction Mechanisms, R. Bruckner, Academic Press, 2002.
6. Organic Chemistry, J. Clayden, N. Greeves, S. Warren, P. Wothers,Oxford University Press, 2004.
7. Mechanism and Theory in Organic Chemistry, T.H. Lowry, K.S. Richardson,2nd Edn.Harper & Row, 1981.
8. Stereochemistry of Organic Compounds: Principles and Applications, D. Nasipuri, 3rd Edn., New Age Pub., 2010.
9. Organic Reaction Mechanisms, V.K. Ahluwalia and Rakesh Kumar Parashar,Narosoa Publishing House, 4thEdn., 2011.
10. Palladium in Heterocyclic Chemistry, Jie Jack Li, Gordon W. Gribble, 2nd Edn.,Tetrahedron Organic Chemistry Series, Volume 26, Elsevier, 2006.
11. Modern synthetic reactions, Herbert O. House, Benjamin-Cummings Publishing Co., 1972.
12. Organic Synthesis, Michael B. Smith, 2nd Edn., McGraw-Hill Higher Education, 2002.

I SEMESTER			
C3	**PHYSICAL CHEMISTRY – I**		**15PCHC13**
Hrs / Week: 5	**Hrs / Sem.: 75**	**Hrs / Unit: 15**	**Credit: 5**

UNIT I: THERMODYNAMICS – I ~~CHEMICAL THERMODYNAMICS~~

Objective*: To have some basic idea about thermodynamics*

Partial Molar quantities – partial molar volume, – chemical potential – physical significance – variation of chemical potential with pressure and temperature – Gibbs Duhem equation – application – chemical potential of a pure solid or liquid and pure ideal gas – thermodynamic function and mixing of ideal gases – ΔG_{mix}, ΔS_{mix}, ΔH_{mix}, ΔV_{mix} and ΔA_{mix} Fugacity – determination of fugacity of a real gas – Physical significance. Activity – concept of activity – activity coefficient – Thermodynamics equation of states – derivation and application – Maxwell's thermodynamics relation.

UNIT II – THERMODYNAMICS – II ~~IRREVERSIBLE THERMODYNAMICS~~

Objective**:** *To have an idea about thermodynamics*

Irreversible Thermodynamics – de Donder treatment of chemical equilibrium – reaction potential – affinity of chemical reaction. Non equilibrium thermodynamics – entropy production – heat flow, matter flow for open system – forces and fluxes – Onsager reciprocal relationship – validity & verification. Thermoelectricity – electro

kinetic and thermomechanical effects – application of irreversible thermodynamics to biological and non linear systems.

UNIT III: PHASE RULE AND COLLOIDS

Objective: *To have an idea about phase rule and colloids*

Three component systems – Graphical representation of ternary system – formation of one pair, two pairs and three pairs of partially miscible liquids, systems composed of two solids and a liquid – ternary solution, hydrate formation – compound formation – method of wet residue – variation of temperature with composition – evolution of a representative point – three component system involving solid phase – salting out.

Colloids: Origin of charge on colloidal particles – electrical double layers theory – Applications of colloids.

~~**CHEMICAL KINETICS I**~~

~~Third order reaction rate – Expression for rate constant for the type A + B+ C → Product (same initial and different initial concentration) – Reversible reaction – Parallel reactions – Consecutive reaction – Chain reaction – Kinetics of H_2 + Br_2 → 2HBr Decomposition of acetaldehyde – Decomposition of ethane – Theory of reaction rate – Lindemann – Activated complex theory – Hinshelwood theory – RRK theory – Marcus theory – RRKM theory.~~

UNIT IV- PHOTOCHEMISTRY

Objective: *To have an idea about photochemistry*

Physical properties of electronically excited molecules – excited molecules – excited state dipole moment – excited state redox potentials – photo physical processes in electronically excited molecules – fluorescence, phosphorescence, internal conversion, intersystem crossing – delayed fluorescence, P – type and E – type – Stern – Volmer equation and its applications – experimental techniques in photochemistry – chemical actinometry and flash photolysis Elementary aspects of photosynthesis.

~~**QUANTUM CHEMISTRY I**~~

~~***Objective:*** *To study about the wave function and its significance*~~

~~Classical wave theory – black body radiation – Planck's quantum hypothesis – Photoelectric effect – Compton effect – Wave – particle duality – de Broglie wave equation – Uncertainty principle – Expression, Experimental proof, outcomes, limitation and Application – Bohr's correspondence principle.~~

~~Schrodinger wave equation – Interpretation and properties of the wave function – significance, orthogonality and nomenclature of the wave function.~~

UNIT V -: QUANTUM CHEMISTRY I

Objective: *To study about the wave function and its significance*

Classical wave theory - black body radiation – Planck's quantum hypothesis – Photoelectric effect – Compton effect – Wave – particle duality – de Broglie wave equation – Uncertainty principle – Expression, Experimental proof, outcomes, limitation and Application – Bohr's correspondence principle.

Schrodinger wave equation – Interpretation and properties of the wave function – significance, orthogonality and nomenclature of the wave function.

~~**QUANTUM CHEMISTRY II**~~

~~Operators – Vector Laplacian – Hermitian – Unity – Projection parity – Ladder operator and density operator – Postulates of Quantum mechanics – Applications of quantum mechanics to the following 1D, 3D box – degeneracy, tunneling, one dimensional Simple Harmonic Oscillator, Rigid rotor.~~

REFERENCES:

1. Physical Chemistry, P. W. Atkins, Oxford University press, 7th Edition, 2002.
2. Physical Chemistry, G. M. Barrow, Tata-McGraw Hill, 5th Edition, 2003.
3. Physical chemistry, G. K. Vemulapalli, Prentice-Hall of India, 1997.
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5. Thermodynamics A Core Course, R. C. Srivastava, S. K. Saha and A. K. Jain, Prentice-Hall of India, II Edition, 2004.
6. Chemical kinetics, Keith J. Laidler, 198, Pearson.
7. Physical Chemistry, Alberty, R.A., and R.S. Silbey and M.G. Bawendi, 4th Edn., Wiley, 2005.
8. A text book of Physical Chemistry, Admason A.W., Academic Press, 1973.
9. Physical Chemistry, Kundu N, and Jain S.K., S. Chand and Co., New Delhi, 1984.
10. Physical Chemistry, Levine, I.N., 5th Edn., Magraw-Hill, 2002.

I SEMESTER			
CE1A	**CHROMATOGRAPHY**		**15PCHE1A**
Hrs / Week: 3	**Hrs / Sem.: 45**	**Hrs / Unit: 9**	**Credit: 3**

UNIT I: CHROMATOGRAPHY-INTRODUCTION

Objective: To study the principle, method and applications of Chromatography

Classification Chromatography methods. Column Chromatography-Principles, experimental procedures, stationary and mobile phases, Choice of Solvent Systems, Separation techniques. Applications

Rf values, Factors affecting R_f values, Experimental procedures, Choice of paper and solvent systems, developments of chromatogram. Detection of the spots. Ascending, Descending and Radial Paper Chromatography, Two Dimensional Chromatography –Applications**.**

UNIT II: **THINLAYER CHROMATOGRAPHY**

Objective: To study the principle and analytical uses of thin-layer chromatography

Principles, factors affecting Rf values. Experimental Procedures. Choice of adsorbents and Solvents.Preparation of plates. Development of the Chromatogram. Detection of the spots. Advantages of thin Layer Chromatography over paper chromatography. Applications

UNIT III: **ION EXCHANGE CHROMATOGRAPHY**

Objective: To study the principle and analytical uses of ion-exchange chromatography

Principle, ion exchange resins and their types- cation exchange resins, anion exchange resins, ion exchange equilibria, properties of ion exchange resins, ion exchange capacity, techniques – applications.

UNIT IV: HIGH PERFORMANCE LIQUID CHROMATOGRAPHY

Objective: *To understand the idea about the High Performance Liquid Chromatography technique.*

Introduction, Instrumentation, Stationary and Mobile Phases.Mobile Phase – Composition. Column – Preparation, Cleaning –regeneration and Storage Conditions. Retention time- Types of HPLC. Applications

UNIT V: GAS CHROMATOGRAPHY

To understand the idea about the Gas Chromatography techniques

Principle, instrumentation choice of injectors, column and detectors - Programmed temperature chromatography, flow programming

chromatography, gas-solid chromatography, and hyphenated techniques in chromatography- Applications of Gas chromatography.

REFERENCES:

1. Fundamentals of Analytical Chemistry – D.A.Skoog, D.M. West, F.J. Holler and S.R. Crouch – 2004; Thompson Asia Private Ltd., Bangalore.
2. Instrumental Methods of Analysis – B. K. Sharma, 2003; Goel publishing House, Meerut.
3. Contemporary Chemical Analysis - Judith F. Rubinson, Prentice Hall (India).
4. Instrumental Methods of Analysis Hobart H. Willard, Lynne L. Merritt Jr, John Dean, Wadsworth Publishing Co Inc; 7th Edn., 1988.
5. Thin Layer Chromatography- A laboratory Handbook, Ashworth, Stahl. E., 1st Edn., Springer-Verlag, 1969.
6. Dynamics of Chromatography - Principles and Theory, J. Calvin Giddings, CRC Press, 2002.
7. Principles of Instrumental Analysis, Douglas A. Skoog, F. James Holler, Stanley R. Crouch, 2006.

I SEMESTER			
CE1B	**BIOCHEMISTRY**		**15PCHE1B**
Hrs / Week: 3	**Hrs / Sem.: 45**	**Hrs / Unit: 9**	**Credit: 3**

UNIT I: CARBOHYDRATES

Objective: *To study about the structure, significance and functions of carbohydrates, Lipids and their derivatives*

Introduction - Definition and Classification of Carbohydrate – Configuration of monosaccharides (glucose, fructose, galactose) – Disaccharides – Structure of maltose, lactose, sucrose – Deoxy sugars – Deoxy ribose – D ribose – Glycosides –physiological significance – amino sugars – importance – Polysaccharides – starch – cellulose – Glycogen – inuline, pectin, chitin.

UNIT II: **AMINO ACIDS AND PROTEINS**

Objective: *To study the important ideas about the structure, functions of amino acids and proteins*

Structure and Classification – abbreviated names (1 letter and 3 letter) – Physical properties of amino acids – chemical properties – codons – Structure and importance of simple peptides like glutathione, Carnosine, anserine, vasopressin – Peptide antibiotics – gramicidine, bacitracine, actinomycin D - Peptide synthesis – Acid chloride method – DCC method – Determination of primary structure of peptide – Identification of N-terminal amino acid – Barger's method – the DNP method – identification of C-terminal amino acid – Hierarchial representation of protein Primary, Secondary, tertiary and quaternary structures – Ramachandran plot.

Structural classification of protein – fibrous, globular and membrane protein.

UNIT III: LIPIDS

Objective: *To study about the structure, significance and functions of Lipids and their derivatives*

Introduction – Classification of lipids – Chemistry of phospholipids – complex lipids – biological functions of phospholipids. Structure and function of Sphingolipids, sphingomycin, cerebroside, gangolioside - Cholesterol – tests, Biochemical functions and physiological significance.

UNIT IV: PURINE, PYRIMIDINE AND NUCLEIC ACIDS

Objective: *To study about the structure, functions and types of nucleic acids.*

Structure of Purines, Pyrimidines – Nucleoside – ribonucleoside, deoxyribonucleosides – nucleotides – ribonucleotides – deoxyribonucleotides – structure and functions of DNA - Watson and

Crick model of DNA- Structure of types of RNA (m-RNA, t-RNA and r-RNA) – Nucleases – structure and function of DNase and RNase – polynucleotides – cyclic nucleotide – structure and function of cAMP, cGMP nucleoprotein – Types of DNA (A-DNA, B-DNA, Z-DNA) – Ramachandran plot

UNIT V: **METABOLISM**

Objective: *To understand about the metabolism process.*

Metabolism – Anabolism ,catabolism - Carbohydrate metabolism – Citric acid cycle – Embden-Meyerhof pathway - Urea cycle – Metabolism of tryptophan. Metabolism of fatty acids – β oxidation – Synthesis of fatty acid synthase.

REFERENCES

1. Biochemistry, Lehinger J.CB S.Publishers,1993.
2. Biochemistry, D.Voet and J.G.Voet. 2nd Edn., John Wiley & Sons. Inc. 1995.
3. Fundamentals of Biochemistry,. Jain J.L Chand & Co. New Delhi, 2000.
4. Biochemistry, Davison, V.L. & Sitlmon, D.L. 4th Edn., Lippinocoth William & Willeing, 1999.
5. Biochemistry, U. Satyanarayana & U. Chakrapani, Books & Allied Pvt. Ltd, 1999.
6. Biochemistry — Lubert Stryer – W. H. Freeman and company, 4th Edn., New York, 1995.
7. Concepts of Biochemistry, A.C. Deb,
8. Biochemistry, S.C. Rastogi, Ane Book (Pvt.) Ltd., 2nd Edn., 2003.
9. Biochemistry, Keshav Trehan, New Age International, 2nd Edn., 1990.
10. Biochemistry Review, U. Satyanarayana, 1st Edn., Arunabaha Sen, 2000.

I SEMESTER		
P I	INORGANIC CHEMISTRY PRACTICAL - I	18PCCH1P1
Hrs / Week: 4	Hrs / Sem.: 60	Credit: 2

I. Inorganic semi-micro qualitative analysis

Analysis of mixture containing two less familiar cations (W, Tl, Se, Te, Mo, Ce, Th, Zr, Ti, V, U, Li)

Minimum 8 mixtures of inorganic compounds should have been analyzed.

II. Complexometric Titrations

1. Estimation of Copper in the presence of Lead
2. Estimation of Zinc in the presence of Barium

REFERENCES:

1. Vogel's Qualitative Inorganic Analysis, 7th edition, Pearson, 2006.
2. College Practical Chemistry, V K Alhuvalia, Sunita Dingra, 1-Edition, University Press, 2005
3. A collection of interesting general chemistry experiments, A. J. Elias, University Press, 2002
4. Inorganic Chemistry Practical, Deepak Pant, e-book, Book Rix edition.

I SEMESTER		
P II	PHYSICAL CHEMISTRY PRACTICAL I	18PCCH1P2
Hrs / Week: 4	Hrs / Sem.: 60	Credit: 2

Conductometric Experiments:

1. Estimation of acetic acid and sodium acetate in the buffer.
2. Estimation of strengths of strong and weak acid in a mixture.
3. Estimation of the strengths of HCl and NH_4Cl in the mixture.
4. Determination of dissociation constant of a weak acid.
5. Determination of solubility product of a sparingly soluble salt.
6. Determination of order of the saponification of an ester by half life method

Potentiometric Experiments:

7. Estimation of FAS by Potentiometric titration
8. Estimation of $KMnO_4$ by Potentiometric titration.
9. Estimation of strengths of strong and weak acid in a mixture by potentiometric method
10. Determination of dissociation constant of a weak acid by potentiometric method

REFERENCES:

1. Experimental Physical Chemistry: A Laboratory Textbook, Arthur Halpern, George McBane, 2006
2. A Manual of Practical Physical Chemistry, Francis William Gray, 2010
3. Physical Chemistry Laboratory Manual, Robb J. Wilson, 2010
4. Practical Physical Chemistry, Alexander Findlay, 2012
5. Physical Chemistry Laboratory, L. Peter Gold, McGraw Hill PVT Ltd., 1997

II SEMESTER			
C4	INORGANIC CHEMISTRY - II		15PCHC21
Hrs / Week: 5	Hrs / Sem.: 75	Hrs / Unit: 15	Credit: 5

UNIT I: COORDINATION CHEMISTRY I

Objective: *To study the fundamentals of coordination chemistry*

IUPAC Nomenclature - Structure and isomerism of the following: Coordination number 1, 2, 3, 4 (tetrahedral, square planar), 5 (Trigonal bipyramidal, Square pyramidal), 6, 7 and 8. Optical, Geometrical isomerism in octahedral complexes – Linkage isomerism.

COORDINATION CHEMISTRY IV

Substitution reaction in octahedral complexes – S_N1, S_N2, S_N1C_B reaction, labile and inert complexes – Interpretation of lability and inertness of transition metal complexes by CFT – Crystal Field Activation Energy (CFAE) with S_N1 and S_N2 reaction – Acid and Base hydrolysis of octahedral complexes.

~~Substitution reaction in square planar complexes – Trans effect – π – bonding theory – Electron transfer reaction – outer sphere and inner sphere mechanism.~~

UNIT II: COORDINATION CHEMISTRY II

Objective: *To have an idea about the crystal field theory and its application.*

Crystal Field theory (CFT)- Important features – Crystal field Splitting of d- orbitals in octahedral, tetragonal, square planar and tetrahedral complexes –Crystal field splitting energy (CFSE) values - factors affecting the value of Δ. Application of crystal field theory in colour, spectral and magnetic properties – Jahn Teller Effect distortion.

~~SPECTRAL PROPERTIES OF COMPLEXES~~

~~Electronic spectra of complexes – LS coupling- j – j coupling - micro state – Term Symbols – Selection rules for electronic transition - Relaxation of spin selection and Laporte selection rule - Orgel diagram for d^1, d^2, d^3, d^4, d^6, d^7, d^8 and d^9 in Octahedral environment – d^6, d^7, and d^8 in tetrahedral environment, Tanabe Sugano diagram - Evaluation of Δ and β values for d^2 (Ti^{2+}) d^7 (Co^{2+}) for octahedral systems and d^3 (V^{2+}), d^8 (Ni^{2+}) tetrahedral systems – Charge transfer spectra for complexes.~~

UNIT III: COORDINATION CHEMISTRY III

Objective: *To study coordination chemistry*

Molecular Orbital Approach- σ and π bonding in octahedral, tetrahedral and square planar complexes.

Electronic and steric effect of complexes, Symbiosis. Thermodynamic stability – stepwise stability constant and overall stability constant – log β value and stability. Factors affecting the stability of complexes in solution – Determination of stability constant by Bjerrum method, spectrometric method and Job's method – comparison of thermodynamic and kinetic stability.

~~METAL CARBONYLS & METAL CLUSTERS.~~

~~Metal carbonyl complexes – Preparation and properties ($Ni(CO)_4$, $Fe(CO)_5$, $Fe_2(CO)_9$, $Cr(CO)_6$, $Re_2(CO)_{10}$), Polynuclear carbonyl complexes ($Fe_3(CO)_{12}$, $Co_4(CO)_{12}$, $Os_4(CO)_{14}$, $Os_4(CO)_{15}$, $Os_4(CO)_{16}$ $Os_5(CO)_{19}$, $Os_6(CO)_{18}$, $Os_6(CO)_{21}$, $Os_7(CO)_{21}$ and $Os_8(CO)_{23}$).~~

~~Carbonyl hydride complexes ($HCo(CO)_4$, $HRe(CO)_5$, $H_2Fe(CO)_4$, $[HCr(CO)_5]^-$, and $HMn(CO)_5$), Isolobal fragments.~~

~~Structure prediction for heteroboranes and organometallic clusters ($B_3H_7[Fe(CO)_3]_2$, $Rh_6(CO)_{16}$), Metal nitrosyls ($Fe(CO)_2(NO)_2$, $Co(CO)_3(NO)$, $Mn(CO)_4(NO)$, $(\eta^5\text{-}C_5H_5)Re(CO)_2NO]^+$ and $Co(NO)(CO)_3$)~~

~~Dinitrogen complexes (Ruthenium and Molybdenum complexes), Metal alkyls, carbenes, carbines and carbides alkyl complexes (Manganese and Iron complexes), carbenes, carbines and carbides complexes (Tungsten and Tantalum complexes), Nonaromatic alkene (Platinum and Nickel complexes) and alkyne complexes (Cobalt~~

~~complex), Allyl and pentadienyl complexes (Manganese and Nickel complexes).~~

~~Metallocenes, Molecular orbitals of Metallocenes.~~

~~Metal clusters – Dinuclear compounds (Rhenium, Molybdenum and Tungsten complexes) – Trinuclear clusters($Re_3Cl_{12}]^{3-}$, Polyatomic zintl anions and cations.~~

UNIT IV: COORDINATION CHEMISTRY IV

Objective: *To study about substitution reaction and metal carbonyls*

Substitution reaction in octahedral complexes – S_N1, S_N2, S_N1CB reaction, labile and inert complexes – Interpretation of lability and inertness of transition metal complexes by CFT – Crystal Field Activation Energy (CFAE) with S_N1 and S_N2 reaction – Acid and Base hydrolysis of octahedral complexes

Substitution reaction in square planar complexes – Trans effect – π - bonding theory – Electron transfer reaction – outer sphere and inner sphere mechanism.

~~**NOBLE GASES, PSEUDOHALOGENS & INTERHALOGEN COMPOUNDS**~~

~~Noble Gas chemistry – Preparation, structure and geometry of Xenon fluorides (XeF_2, XeF_4, XeF_6) – Structure of oxy fluorides of xenon ($XeOF_2$, $XeOF_4$, XeO_2F_2, XeO_3F_2, XeO_3F_4).~~

~~Halogens - Iodine – Basic properties – evidences.~~

~~Pseudohalogens – Structure, preparation, properties and uses of $(CN)_2$, $(SCN)_2$, $(SeCN)_2$.~~

~~Interhalogen compounds Preparation, properties, structure and uses of ICl, IBr, BrF_3, ICl_3, ClF_3, IF_5, IF_7.~~

~~Polyhalide ions and polyhalides – classification – preparation properties. Structure and shape of ICl_2^-, ICl_2^+, ICl_4^-, IF_4^+ and higher polyhalide ions. Similarities and dissimilarities between halogens and pseudohalogens, halide ions and pseudohalide ions.~~

UNIT V: SPECTRAL PROPERTIES OF COMPLEXES

Objective*: To have some idea spectral properties of complexes*

Electronic spectra of complexes – LS coupling- j – j coupling - micro state –Term Symbols – Selection rules for electronic transition - Relaxation of spin selection and Laporte selection rule - Orgel diagram for d^1, d^2, d^3, d^4, d^6, d^7, d^8 and d^9 in Octahedral environment – d^6, d^7, and d^8 in tetrahedral environment, Tanabe Sugano diagram - Evaluation of Δ and β values for d^2 (Ti^{2+}) d^7 (Co^{2+}) for octahedral systems and d^3 (V^{2+}), d^8 (Ni^{2+}) tetrahedral systems - Charge transfer spectra for complexes.

~~**NUCLEAR CHEMISTRY**~~

~~Thermal and nuclear reactions, Q value, capture cross section, threshold energy and excitation functions. Types of nuclear reactions – spallation, fission and fusion – Fissile and Fertile isotopes. Nuclear fission – characteristics – product distribution – theories of fission (liquid drop model only) – Nuclear fusion and stellar energy, nuclear~~

~~reactors – nuclear materials and waste disposal. Radiation hazards and protection, atomic power projects in India.~~

~~Hydrated electrons: Hart and Boag's experiment for producing hydrated electrons, other methods of obtaining hydrated electrons, Properties.~~

REFERENCE BOOKS:

1. Principles of Inorganic Chemistry, Puri Sharma. Vishal Publishers, 2008.
2. Inorganic Chemistry - Principles, Structure and Reactivity, J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi,4th Edn., Pearson Education, 2006
3. Concise Inorganic Chemistry, J. D. Lee, Elbs with Chapman and Hall, London
4. Advanced Inorganic Chemistry, F. A. Cotton, G. Wilkinson, C.A. Murillo & M. Bochmann, 6th Edn., Wiley India Pvt. Ltd., 2014.
5. Advanced Inorganic Chemistry, Satyaprakash, G.D. Tuli and S.K. Basu., Volume 1, S. Chand and Company, 2006
6. Modern Inorganic Chemistry, Willam L. Jooly, Magraw-Hill, 1991.
7. Physical Methods in Chemistry, R S Drago, W B Saunders, 1977
8. Inorganic Chemistry, D. F. Shriver and P.W. Atkins, 4th Edn., Harper Collins, 1993.
9. Modern Inorganic Chemistry, R. D. Madan & Satya Prakash, S Chand and Company, Ltd., 1st Edn., 1987.
10. Inorganic Chemistry, Gary L. Miessle and Donald A. Tarr, Dorling Kindersley (India) Pvt. Ltd., 3rd Edn., 2009
11. Structural methods in Inorganic Chemistry, E A V Ebsworth, David, W H Rankin, Sleptren Credock, Blackwell; 2nd Edn., 1991.
12. Advanced Inorganic Chemistry, F. A.Cotton , 5th edition.
13. Physical Inorganic Chemistry- A Coordination Approach,S.F.A. Kettel, Oxford University Press; New edition, 1998.

II SEMESTER			
C5	**ORGANIC CHEMISTRY II**		**15PCHC22**
Hrs / Week: 5	**Hrs / Sem.: 75**	**Hrs / Unit: 15**	**Credit: 5**

UNIT I: STEREOCHEMISTRY

***Objective*:** *To have an idea about stereochemistry*

Chirality – prochirality – enantiotopic and diastereotopic atoms – ~~Fischer, Wedge, Newmann and Sawhorse formulas~~, RS, EZ notation – racemization – Walden inversion - Planar chirality in paracyclophanes and ANSA compounds – Stereoselective and stereospecific Reactions – Asymmetric synthesis – Cram's Rule, Prelogs Rule, Cram's chelation model and Felkin Ahn model – Newman projection formula – Sawhorse formula – Geometrical isomers-Methods of determining geometrical isomerism - Conformational analyses of mono and disubstituted cyclohexanes – Effect of conformation on the physical properties and the reactivity of acylic and cyclohexane systems. ~~ethane, butane, ethylene glycol, dibromo butane, cyclohexane (1,2 dimethyl, 1,3 dimethyl, 1,4 dimethyl cyclohexane), 1,2 Disubstituted cyclohexanes with two different substituents.~~

UNIT II: AROMATICITY, NOVEL RINGS

Objective*: To have some idea about aromaticity and novel rings*

a Aromaticity: Benzenoid and non-benzenoid aromatic compounds – Huckel's rule – concept of aromaticity, homo-aromaticity and anti-aromaticity – Systems with 2,4,6,8 and 10 electrons - Annulenes – fulvene, azulenes, tropolones

b. Novel rings: Nomenclature of bicyclic and tricyclic systems- Adamantane and cubane.

c. Fullerenes, Benzocorannulenes, Catenanes, Rotaxanes Cucurbit[n]uril-Based Gyroscane- structure.

~~**SOME NAME REACTIONS IN ORGANIC CHEMISTRY:**~~

~~Mechanism and their applications in organic synthesis - Aldol condensation, Arndt – Eistert synthesis, Benzoin condensation, Cannizaro reaction, Mannich reaction, Reformatsky reaction, Clemmensen reduction, Kolbe Schmitt Reaction, Schotten Baumann Reaction, Friedel-Crafts Acylation, Friedel-Crafts Alkylation. Swern Oxidation (DMSO/ Dichloromethane).~~

~~Coupling Reactions: Heck reaction, Sonogashira coupling, Suzuki reaction.~~

UNIT III: HETEROCYCLIC CHEMISTRY

Objective: *To study about a few heterocyclic compounds*

Quinoline- Skraup synthesis, Friedlander's Synthesis, and reactions, Isoquinoline – Bischler Napieralski reaction, Pomeranz – Fritsch Reaction – Indole- Fischer Indole synthesis – Madelung Synthesis reactions.

Structure synthesis and reactions of oxazole, imidazole, thiazole, coumarins, flavones, isoflavones, cyanin, anthocyanins, α-pyrones, γ-pyrones, chromones, caffeine, theobromine and theophylline.

UNIT IV: ALKALOIDS & TERPENOIDS

Objective: *To study about alkaloids* & terpenoids

Alkaloids: Occurrence, Classification, Structural elucidation and synthesis of quinine, nicotine, morphine, lysergic acid and reserpine.

Terpenoids: Classification – Isoprene rule, Structural elucidation of citral, camphor α-pinene, zingiberne and abietic acid.

~~**PHOTOCHEMISTRY**~~

~~Thermal and Photochemical reaction – allowed and forbidden transition Jablonski diagram – Photo sensitization – Photochemistry of excited ketones (acetone, 2 hexanone, benzophenone) Norrish type I & II reaction – Paterno Buchi reaction – Di π methane rearrangement – Photo reduction – Photochemistry of olefins – cis & trans isomerization.~~

UNIT V: ORGANIC PHOTOCHEMISTRY

***Objective**: To have some idea about photochemistry*

Thermal and Photochemical reaction – allowed and forbidden transition- Jablonski diagram, Phosphorescence, fluorescence – Photo sensitization – Photochemistry of excited ketones (acetone, 2-hexanone, benzophenone)-Norrish type I & II reaction – Paterno Buchi reaction – Di π methane rearrangement – Photo reduction – Photochemistry of olefins – cis & trans isomerization

~~**MOLECULAR REARRANGEMENT**~~

~~Rearrangement involving migration of electron deficient carbon – Pinacol – pinacolone rearrangement – Baeyer Villiger Rearrangement – Wolff rearrangement – Benzil- Benzilic acid rearrangement.~~

~~Rearrangement involving migration of electron deficient nitrogen – Beckmann rearrangement – Lossen rearrangement – Schmidt rearrangement.~~

~~Rearrangement involving migration of electron deficient oxygen – Dakin reaction.~~

~~Rearrangement involving migration to electron rich carbon – Favorski rearrangement – Sommelet Hauser rearrangement.~~

~~Aromatic rearrangement – Hoffmann – Martius rearrangement~~

~~Rearrangement involving migration of oxygen to ring – Fries rearrangement – Sigmatropic rearrangement – Claisen rearrangement~~

REFERENCE BOOKS

1. Stereo Chemistry Of Carbon Compounds, E L Elliel, McGraw Hill 1999
2. Introduction to Stereochemistry, K. Mislow, W. A. Benjamin, New York, 1966.
3. Stereo Chemistry, V M Potapov, MIR publications 1979

4. Stereo Chemistry – Conformation and Mechanism, Kalsi, New Age International (P) Ltd 2000
5. Advanced Organic Chemistry, 4th Edn., Jerry March, 1992
6. Organic Chemistry, I L Finar, Vol II ELBS, 5th Edn, 2000
7. A Guide Book To Mechanism In Organic Chemistry, P. Sykes, Orient Longman, 1989
8. Fundamentals Of Organic Reaction Mechanism, J M Harris and C Wamser, 1st Edn., John, Wiley and Sons, 1976.
9. Reaction Mechanism In Organic Chemistry, S M Mukherji and S P Sing, Macmillan India Ltd., 2009.
10. Organic chemistry, Paula Yurkanis, 3rd Edn, Pearson Education Asia 2002

II SEMESTER			
C6	**PHYSICAL CHEMISTRY – II**		**15PCHC23**
Hrs / Week: 5	**Hrs / Sem.: 75**	**Hrs / Unit: 15**	**Credit: 5**

UNIT I – CHEMICAL KINETICS – I

***Objectives**: To study about various theories of reaction rate*

Third order reaction rate – Expression for rate constant for the type A + B+ C → Product (same initial and different initial concentration) – Reversible reaction – Parallel reactions – Consecutive reaction – Chain reaction –Kinetics of $H_2 + Br_2 \rightarrow 2HBr$ Decomposition of acetaldehyde – Decomposition of ethane – Theory of reaction rate – Lindemann – Activated complex theory – Hinshelwood theory – RRK theory – Marcus theory – RRKM theory.

~~**PHASE RULE AND COLLOIDS**~~

~~Three component systems – Graphical representation of ternary system – formation of one pair, two pairs and three pairs of partially miscible liquids, systems composed of two solids and a liquid – ternary solution, hydrate formation – compound formation – method of wet residue – variation of temperature with composition – evolution of a representative point – three component system involving solid phase – salting out.~~

~~Colloids: Origin of charge on colloidal particles – electrical double layers theory – Applications of colloids.~~

UNIT II: ELECTROCHEMISTRY – I

***Objectives**: To know the theory and various models involved in electrochemistry*

Debye – Huckel theory of strong electrolytes – Activity coefficient of electrolytes –activity coefficient – ionic strength – Debye Huckel theory of mean ionic activity coefficient ~~Debye Huckel Limiting Law – derivation and verification~~ – Determination of solute activities from solvent activities – Bjerrum's theory of ion association in electrolyte solution – Electrified interfaces – thermodynamic treatment – electrical capacitance. Determination of the surface excess – Structure of the electric field – Helmholtz – Perrin Model, Gouy – Chapmann diffusion model and Stern Model.

UNIT III : ELECTROCHEMISTRY – II

***Objectives**: To have an idea about the advanced concepts in electrochemistry*

Kinetics of electrode reaction – Buttler Volmer equation – Tafel equation – Diffusion over potential. Irreversible electrode process – Overvoltage – Applications – electro deposition – corrosion – Polarography – Concentration potential – DME assembly – Advantages – Ilkovic equation – Derivation – Half –wave potential – Amperometric and coloumetric titration.

UNIT IV: QUANTUM CHEMISTRY II

***Objective:** To understand the operators applied in quantum chemistry*

Operators – Vector- Laplacian – Hermitian – Unity – Projection parity - Ladder operator and density operator – Postulates of Quantum mechanics – Applications of quantum mechanics to the following 1D, 3D box – degeneracy, tunneling, one dimensional Simple Harmonic Oscillator, Rigid rotor.

~~**GROUP THEORY I**~~

~~Group theory – Symmetry elements – symmetry operations – Postulates of Group Point groups – C_p, C_{2v}, C_{3v}, C_{2h}, D_2, D_6, D_{2d}, D_{2h} – Determination of Point groups – Representation of molecular point groups – reducible representation and irreducible representation – Great orthoganality theorem (GOT) – Use of GOT to construct character tables – character tables for point groups – C_{2v}, C_{3v},C_{2h},D_{3h}~~

UNIT V: QUANTUM CHEMISTRY III

Objective: *To understand in detail about importance of spin-orbit interactions for atoms.*

Hydrogen atom – Radial distribution function – Angular part of the wave function – Electron spin – Quantum numbers-

Wave function of many electron systems – Helium atom - Pauli's exclusion principle – Slater determinants – Angular Momentum - Commutators relations – step-up and step-down operators - angular momentum in many electron atom – Spin – orbit interaction.

~~**GROUP THEORY II**~~

~~Reducible representation into its irreducible representation – Rules for determining the irreducible representation of Vibrational modes normal modes of vibration of polyatomic molecules H_2O – NH_3,BF_3 Direct product of irreducible representation selection rule for the n π^*& π π^* transition in HCHO construction of Hybrid orbitals – CH_4, $[PtCl_4]^{2-}$ secular equation in MO theory-trans 1,3-butadiene, Benzene.~~

REFERENCES:

1. Fundamentals of Photochemistry, K.K. Rohatgi- Mukherjee, Wiley- Eastern, New Delhi, 1978.
2. Principles and Applications of Photochemistry, Wayne, R.P., Oxford University Press, 1988.
3. Principles and Applications of Electrochemistry, Crow, D.R., Chapman and Hall, 1988.
4. Electrochemistry, Reiger, P.H., Chapman and Hall, 2nd Edn., 1983.
5. Statistical Mechanics, Gopal, E.S.R, Macmillan (India) Ltd., New Delhi, 1974.
6. Statistical Mechanics, Davidson, N., McGraw-Hill, 1962.
7. Group Theory in Chemistry, Gopinathan, M.S., and V. Ramakrishnan, Vishal Publications, Jalandhar (India), 1986.
8. Group Theory and Applications in Chemistry, Raman, K.V., Tata McGraw-Hill, New Delhi, 1990.
9. Group Theory and Symmetry in Chemistry, Hall, L.H., McGraw-Hill, 1969.

10. Group Theory and Applications to Quantum Mechanics of Atomic Spectra, Academic Press, 1959.
11. Physical Chemistry, Peter Atkins and Julio de Paula, W. H. Freeman and Company, 8th edition, 2006.

II SEMESTER			
CE2A	**INSTRUMENTAL METHODS OF ANALYSIS**		**15PCHE2A**
Hrs / Week: 3	**Hrs / Sem.: 45**	**Hrs / Unit: 9**	**Credit: 3**

UNIT I - THERMOANALYTICAL METHODS

Objective: *To study the analytical uses of thermal analytical methods*

Thermo Gravimetric Analysis (TGA) – principle, instrumentation, application - Factors affecting TGA -Differential Thermal Analysis (DTA) – principle and instrumentation, DTA of Calcium oxalate monohydrate – Comparison of DTA - TGA curves.

UNIT – II - ELECTRO-ANALYTICAL METHODS

Objective: *To study the analytical uses of electro analytical methods*

Electro Gravimetric Analysis (EGA) – theory, types of EGA, instrumentation and applications in the estimation of metal ions in solution. Polarography – principle – dropping mercury electrode (DME). Advantages of DME- applications

UNIT III: COLORIMETRIC, SPECTROPHOTOMETRIC ANALYSIS , IR & RAMAN spectroscopy

Objective: *To study the principle and instrumentation of colorimetry , UV-visible spectrophotometer , IR and Raman spectroscopy*

Visible colorimetry – Principle, instrumentation –Applications. Spectrophotometer- instrumentation- Applications -UV-VIS Spectrophotometer – Single beam and Double – beam Spectrometer - Applications – IR spectrometer- theory, principle, instrumentation sampling techniques- factors influencing vibrational frequencies Applications. Raman spectroscopy-Raman Effect Conditions for Raman spectrum, Instrumentation – Comparison between IR and Raman Spectroscopy.

UNIT IV: FLUOROMETRY, FLAME AND NEPHLOMETRY ANALYSIS

Objective: *To study the principle and instrumentation of flame photometry*

Fluorometry – principle – instrumentation and applications. Flame photometry – principle – instrumentation and applications. Nephelometry and turbidimetry - theory - instrumentation and applications. Atomic Absorption Spectroscopy- Principle, Instrumentation- Spectral and Chemical Interferences-Applications.

UNIT V: NMR, PHOTOELECTRON SPECTROSCOPY AND MEDICAL IMAGING TECHNIQUES

Objective: *To study the principle and instrumentation of NMR and PES and medical imaging techniques*

NMR spectroscopy, - Principle and Instrumentation. Applications. Photoelectron Spectroscopy – principle – Instrumentation. Medical Imaging- Magnetic Resonance Imaging (MRI) Positron emission

tomography (PET) , Single-photon emission computed tomography (SPECT). Computer-assisted tomography (CT) , Echocardiography- Basic theory and Applications

REFERENCES:

1. Fundamentals of Analytical Chemistry – D.A.Skoog, D.M. West, F.J. Holler and S.R. Crouch – 2004; Thompson Asia Private Ltd., Bangalore.
2. Instrumental Methods of Analysis – B. K. Sharma, 2003; Goel publishing House, Meerut.
3. Contemporary Chemical Analysis - Judith F. Rubinson, Prentice Hall (India).
4. Instrumental Methods of Analysis Hobart H. Willard, Lynne L. Merritt Jr, John Dean, Wadsworth Publishing Co Inc; 7th Edn., 1988.
5. Thin Layer Chromatography- A laboratory Handbook, Ashworth, Stahl. E., 1st Edn., Springer-Verlag, 1969.
6. Dynamics of Chromatography - Principles and Theory, J. Calvin Giddings, CRC Press, 2002.
7. Spectroscopy of organic compounds, Kalsi, P.S., New Age Publishers New Delhi, 2007.
8. Principles of Instrumental Analysis, Douglas A. Skoog, F. James Holler, Stanley R. Crouch, 2006.
9. Fundamentals of Medical Imaging, Paul Suetens, 2nd Edition, Cambridge University Press, 2002.

II SEMESTER			
DSE2A	APPLIED CHEMISTRY		18PECH2A
Hrs / Week: 4	Hrs / Sem.: 60	Hrs / Unit: 12	Credit: 4

UNIT I: FUEL CELLS

Introduction, General chemistry of fuel cells, Hydrogen-oxygen fuel cells, Hydrocarbon oxygen fuel cells, Carbon monoxide fuel cell, Methyl alcohol fuel cell, Hydrogen oxygen cells in manned space flights, Efficiency of fuel cells, Advantages of fuel cells, Fuel cells The future of clean energy.

UNIT II: FERMENTATION

Introduction, historical, conditions favorable for fermentation, Characteristics of enzymes, short account of some fermentation processes, Manufacture of spirits, Manufacture of vinegar, Manufacture of power alcohol, Ethyl alcohol from molasses, preparation of wash, Distillation, Alcohol from waste sulphite liquor, Manufacture from starchy materials, Manufacture from cellulose materials, Manufacture from hydrocarbon gases, Importance of power alcohol as a fuel, Distillery effluents for agricultural production.

UNIT III: OILS, FATS AND WAXES

Oils and fats: Introduction, Distinction between oils and fats, properties, classification, vegetable oils, Manufacture of cotton seed oil by expression and solvent extraction, Manufacture of soya bean oil by solvent extraction, Refining of crude vegetable oils, some other vegetable oils, Animal oils, Animal fats and oils, processing of animal fats and oils, Mineral oils, Difference between animal, vegetable and mineral oils.

Waxes: classification, properties, some common waxes, Synthetic oils, fats and waxes, Analysis of oils, fats and waxes, Saponification value, Ester value, Acid value, Iodine value, Wijs method, Reichert Meissl method, Henher value, Elaiden test, Aniline point, manufacture of candles.

UNIT IV: INSECTICIDES

Introduction, Inorganic insecticides, Natural or plant insecticides, Organic insecticides, DDT, BHC, Gammexane, Aldrin and dieldrin, Endrin, Attractants and repellents, fumigants, Miticides, Rodenticides, Fungicides, Herbicides, Acaricides, Synthetic insecticides, Pesticides pollution, Persistent pesticides, Biological magnification, Biodegradation of pesticides, Mode of poisoning of pesticides, The degradation and mobility of pesticides.

UNIT V: PAINTS AND PIGMENTS

Pigments: Introduction, white pigments, white lead, characteristics of the pigment, uses, Zinc oxide, characteristics of the pigment, uses, Titanium dioxide, characteristics of the pigment, uses, Blue pigments, ultramarine blue, uses, cobalt blues and iron blues, uses, red pigments, characteristics of the red lead, uses, synthetic iron oxide pigment, uses, green pigments, chrome green, uses, black pigments, yellow pigments, Tonners, Metallic powders as pigments.

Paints: Classification of paints, constituents of paints, Requirements of a good paint, Importance of PVC, paint failure,

Emulsion paints constituents of emulsion paints, Advantages, Latex paints, Luminescent paints, Fire retardant paints, Heat resistant paints.

REFERENCE BOOKS:

1. Industrial Chemistry – B.K.Sharma, 2003, Goel Publishing House, Meerut.
2. Industrial Chemicals – Faith etal, Wiley Interscience, New York.
3. Chemical Process Industries – R.N. Shreve, 2000; Tata McGraw Hill Publishing Company, Mumbai.
4. Text Book of Pharmaceutical Chemistry – Jaysgree Ghosh, 2003; S. Chand and Company, New Delhi.
5. Fundamentals of Analytical Chemistry – D.A.Skoog, D.M. West, F.J. Holler and S.R. Crouch – 2004; Thompson Asia Private Ltd., Bangalore.

II SEMESTER			
CE2B	**ENZYME CHEMISTRY**		**15PCHE2B**
Hrs / Week: 3	**Hrs / Sem.: 45**	**Hrs / Unit: 9**	**Credit: 3**

UNIT I: ENZYME - INTRODUCTION

Objective: *To understand classification, nomenclature and purification of enzyme*

Enzyme Classification and nomenclature – isolation and purification properties of enzymes – enzyme specificity effect of pH, temperature, concentration of enzyme, concentration of substrate on enzyme activity and stability – units of enzyme activity and stability – co-enzymes and co-factors.

UNIT II: KINETICS AND MECHANISM OF ENZYME CATALYZED REACTION

Objective: *To understand the kinetics and mechanism of enzyme catalyzed reaction*

Induced fit reaction – Lock and key mechanism - Kinetics and mechanism of enzyme catalysed reaction – Steady state kinetics – Derivation of Michealis-Menton equation – significance of V_{max} and k_m– L–plot – Multistage enzyme kinetics – pre-steady state relaxation kinetics – King and Allman procedure – Negative and positive cooperativity (feedback inhibition) – enzyme inhibition – enzyme immobilization and its application.

UNIT III: MECHANISM OF ENZYMES AND TYPES

Objective: *To understand the mechanism of enzyme reaction and other types of enzymes*

Active sites – Mechanism of enzyme action – lysoyme, chymotrypsin, DNA polymerase RNAse, isoenzymes (IDH), allosteric enzyme, ribozyme & abzyme.

UNIT IV: MULTI ENZYME COMPLEX

Objective: *To have an idea about the multi enzyme complex advantage and biosensors*

Multienzyme complexes – structure and function of pyruvate dehydrogenase and fatty acid synthase complex – Advantages of multienzyme complex – Commercial application of enzymes in food pharmaceutical and other industries – enzymes for diagnostic applications – Biosenors

UNIT V: EXTREMOZYMES

Objective: *To have an idea about Extremozymes and industrial applications*

Extremozymes – Extremophiles – Thermophiles – Halophiles – Psychrophiles – Industrial application – protein engineering (site – directed mutagenesis).

REFERENCES

1. Biochemistry, Lehinger, J., CBS. Publishers, 1993
2. Biochemistry, D.Voet and JG, Voet, John Wiley & Sons, Inc. 2nd Edn., 1995.
3. Fundamentals of Biochemistry, Jain J.L Chand & Co, New Delhi, 2000
4. Biochemistry, Davison, V.L. & Sitlmon, D.L. 4th Ed, Lippinocoth William & Willeing, 1999
5. Enzymolgy, Malcom Dixon and Edwin C. Webb Academic Press, 2nd Ed. edition 1964
6. Enzyme Technology, Martin Chaplin, Christopher Bucke, Cambridge University Press, 1990
7. Enzyme Technology, Ashok Pandey, Colin Webb, Carlos Ricardo Soccol, Christian Larroche, Asiatech Publishers Inc., 2005
8. Enzyme Technology, S. Shanmugham, I. K. International Pvt. Ltd., 2009
9. Enzymology and Enzyme Technology, S.M. Bhatt, S. Chand, 2011
10. Enzyme Technology, Anusha Bhaskar, V.G. Vidhya, MJP Publishers, 2009

II SEMESTER			
DSE2B	CHEMINFORMATICS		18PECH2B
Hrs / Week: 4	Hrs / Sem.: 60	Hrs / Unit: 12	Credit: 4

UNIT I: COMPUTER REPRESENTATION AND MANIPULATION OF 2D MOLECULAR STRUCTURE

Scope of Cheminformatics Computer – Representations of Chemical Structures, Graph Theoretic Representations of Chemical Structures, Connection Tables and Linear Notations, Canonical Representations of Molecular Structures – Structure Searching Screening Methods, Algorithms for Subgraph Isomorphism, Practical Aspects of Structure Searching.

UNIT II: INTRODUCTION TO DATABASES & ITS CLASSIFICATION

Characteristics and categories of databases – Sequence databases – Nucleotide sequence databases – EMBL, DDBJ, GenBank – Secondary nucleotide sequence databases – UniGene, STACK, Ribosomal databases, HIV sequence database, REBASE – Protein sequence databases – UniProtKB, SWISSPROT, TremBL, PDB.

UNIT III: DATABASES AND DATA SOURCES IN CHEMISTRY

Classification of databases – Literature databases – Chemical Abstracts System (CAS) – SCISEARCH & MEDLINE – Factual databases – property databases – Beilstein and Gmelin – Crystal structure databases – CSD, ICSD– Structure databases – NCI – Chemical reaction databases – Classification of Scientific Literature – primary, secondary and tertiary literature – Online databases – access to CAS with SciFinder Scholar 2002.

UNIT IV: CHEMICAL INFORMATION SEARCHES & STRUCTURE DESCRIPTORS

Full structure search – Substructure search – Backtracking algorithm – Screening – similarity search –similarity measure – Tanimato – 3D structure search.

Descriptors Definition – classification – structure keys – topological description – 3 D descriptors – chirality descriptors – Conformation independent and conformation dependent.

UNIT V: APPLICATIONS OF CHEMINFORMATICS

Prediction of properties – estimation of log Pw, log S & Toxicity prediction of spectral properties – chemical shift, IR simulation and mass spectra – prediction of chemical reactions – computer assisted synthesis design – Drug design – target identification & validation – lead finding and optimization – design of combinatorial libraries – Structure based and ligand based drug design

REFRENCES:

1. Computational Molecular Biology, Pevzner, P.A, Prentice Hall of India Ltd, New Delhi, 2004.
2. Bioinformatics and Functional Genomics, Pevsner, J., John Wiley and Sons, New Jersey, USA, 2003.
3. Bioinformatics: Sequence and Genome Analysis, Mount, D), Cold Spring Harbor Laboratory Press, New York, 2004.

4. Bioinformatics – a practical guide to the analysis of Genes and Proteins, Baxevanis, A.D. and Francis Ouellellette, B.F.(), John Wiley & Sons, UK, 1998.
5. Molecular Modeling, Principles and Applications, II Edition, Andrew R. Leach, Dorset Press, Dorchester, Dorset, 2001.
6. Cheminformatics, ed., Johann Gasteiger and Thomas Engel, Wiley VCH, Weineim, 2003.
7. Introduction to Chemiformatics, Andrew.R. Leach and Valeric J Gillet, Springer, 2007.

I & II SEMESTER			
CP1	INORGANIC CHEMISTRY PRACTICAL - I		15PCHC2P1
Hrs / Week: 4	Hrs / Sem.: 60	Hrs / Year: 120	Credit: 3

I. Inorganic semi-micro qualitative analysis

a. Analysis of mixture containing two less familiar cations (W, Tl, Se, Te, Mo, Ce, Th, Zr, Ti, V, U, Li)

II. Complexometric Titrations

1. Estimation of Copper in the presence of Lead
2. Estimation of Zinc in the presence of Barium

III. Chromatographic techniques

Separation of mixtures

(i) Cadmium and Zinc

(ii) Zinc and Magnesium

TLC separation of Ni, Mn, Co and Zn. Determination of R_f values.

REFERENCES:

1. Vogel's Qualitative Inorganic Analysis, 7th edition, Pearson, 2006.
2. College Practical Chemistry, V K Alhuvalia, Sunita Dingra, 1-Edition, University Press, 2005
3. A collection of interesting general chemistry experiments, A. J. Elias, University Press, 2002
4. Inorganic Chemistry Practical, Deepak Pant, e-book, Book-Rix edition.

I & II SEMESTER			
CP2	ORGANIC CHEMISTRY PRACTICAL – I		15PCHC2P2
Hrs / Week: 4	Hrs / Sem.: 60	Hrs / Year: 120	Credit: 3

I. Separation and organic qualitative analysis of the mixture containing one or two functional group. The students are expected to determine the physical constants for both the components and their derivatives.

II. Organic preparation:

1 Preparation of p-acetotoluidide from p-toluidine
2 Preparation of benzoylglycine from glycine
3 Preparation of 1,2,3,4-tetrahydrocarbazole from cyclohexanone
4 Preparation of p-Benzoquinone from hydroquinone
5 Preparation of p-Bromoaniline from acetanilide
6 Preparation of m-nitrobenzoic acid from methyl benzoate
7 Preparation of p-nitroaniline from acetanilide
8 Preparation of benzpinacolone from benzophenone (Course work)
9 Preparation of benzanilide from benzophenone (Course work)
10 Preparation of tribromobenzene from aniline (Course Work).

REFERENCE BOOKS:

1. Practical Organic Chemistry Floyd George Mann, Frederick George Mann, Bernard Charles Saunders, Longmans, 1962.
2. Comprehensive Practical Organic Chemistry, V K Ahluwalia and Sunita Dhingra, Universities Press (India) Private Limited, 2000.
3. Vogels Text book of Practical Organic Chemistry, B.S. Furniss, A.J. Hannaford, V, Rogers, R.W.G. Smith, and A.R. Tatchell, ELBS.
4. Understanding the Principles of Organic Chemistry: A Laboratory course: Peterson Myres, Cengage Learning, 2010.
5. Laboratory Manual of Organic Chemistry, Raj K Bansal, New Age International, 2009.
6. A Manual of Organic Chemistry Practical, Practical and Theoretical, Huge Clement, W.G. Blackie and Co Printers, 1879.
7. Practical Organic Chemistry, 4th Edn., F G Mann , S C Saunders, 1978.

I & II SEMESTER			
CP3	PHYSICAL CHEMISTRY PRACTICAL		15PCHC2P3
Hrs / Week: 4	Hrs / Sem.: 60	Hrs / Year: 120	Credit: 3

Conductometric Experiments:

1. Estimation of acetic acid and sodium acetate in the buffer.
2. Estimation of strengths of strong and weak acid in a mixture.
3. Estimation of the strengths of HCl and NH_4Cl in the mixture.
4. Determination of dissociation constant of a weak acid.
5. Determination of solubility product of a sparingly soluble salt.
6. Determination of order of the saponification of an ester by half-life method
7. Determination of rate constant of the saponification of an ester
8. Determination of activity coefficients of zinc ions in the solution of 0.002 M $ZnSO_4$ using Debye Huckel Limiting law.

Potentiometric Experiments:

9. Estimation of FAS by Potentiometric titration
10. Estimation of $KMnO_4$ by Potentiometric titration.
11. Estimation of strengths of strong and weak acid in a mixture by potentiometric method
12. Determination of dissociation constant of a weak acid by potentiometric method
13. Determination of thermodynamic constants ΔG, ΔS and ΔH for the reaction by emf method.

REFERENCES:

1. Experimental Physical Chemistry: A Laboratory Textbook, Arthur Halpern, George McBane, 2006
2. A Manual of Practical Physical Chemistry, Francis William Gray, 2010
3. Physical Chemistry Laboratory Manual, Robb J. Wilson, 2010
4. Practical Physical Chemistry, Alexander Findlay, 2012
5. Physical Chemistry Laboratory, L. Peter Gold, McGraw-Hill PVT Ltd., 1997

~~II SEMESTER~~		
~~P III~~	~~ORGANIC CHEMISTRY PRACTICAL – I~~	~~18PCCH2P1~~
~~Hrs / Week: 4~~	~~Hrs / Sem.: 60~~	~~Credit: 2~~

~~**QUALITATIVE ANALYSIS AND ORGANIC PREPARATION**~~

I.Separation and organic qualitative analysis of the mixture containing one or two functional group. The students are expected to determine the physical constants for both the components and their derivatives.

Minimum 8 mixtures of organic compounds should have been analyzed

II. Organic preparation [Single Stage preparation]:

1. Preparation of Phenyl hydrazone from cyclohexanone
2. Preparation of p-Benzoquinone from hydroquinone
3. Preparation of resacetophenone from resorcinol
4. Preparation of dinitrophenylamine from aniline
5. Preparation of benzpinacol from benzophenone
6. Preparation of methyl-m-nitrobenzoate from methyl benzoate
7. Preparation of benzophenone oxime from benzophenone
8. Preparation of tribromobenzene from aniline.

REFERENCE BOOKS:

1. Practical Organic Chemistry Floyd George Mann, Frederick George Mann, Bernard Charles Saunders, Longmans, 1962.
2. Comprehensive Practical Organic Chemistry, V K Ahluwalia and Sunita Dhingra, Universities Press (India) Private Limited, 2000.
3. Vogels Text book of Practical Organic Chemistry, B.S. Furniss, A.J. Hannaford, V, Rogers, R.W.G. Smith, and A.R. Tatchell, ELBS, 2003.
4. Understanding the Principles of Organic Chemistry: A Laboratory course: Peterson Myres, Cengage Learning, 2010.
5. Laboratory Manual of Organic Chemistry, Raj K Bansal, New Age International, 2009.
6. A Manual of Organic Chemistry Practical, Practical and Theoretical, Huge Clement, W.G. Blackie and Co Printers, 1879.
7. Practical Organic Chemistry, 4th Edn., F G Mann , S C Saunders, 1978.

II SEMESTER		
P-IV	CHROMATOGRAPHY PRACTICAL	18PCCH2P2
Hrs / Week: 4	Hrs / Sem.: 60	Credit: 2

Chromatographic techniques

Separation of mixtures

1. Aniline and m-nitro toluene
2. Benzophenone and benzoic acid and checking their R_f values.
3. Identification of amino acid with the help of TLC or PC. Calculation of R_f value of individual amino acid.
4. Identification of sugar (glucose, fructose, sucrose) with the help of TLC or PC. Calculation of R_f value.
5. Paper chromatographic separation of Cadmium and Zinc. Determination of R_f values.
6. Paper chromatographic separation of red and blue inks. Determination of R_f values.
7. TLC separation of Mn and Zn. Determination of R_f values.
8. TLC separation of Ni and Co. Determination of R_f values.

REFERENCES:

1. Vogel's Qualitative Inorganic Analysis, 7th edition, Pearson, 2006.
2. College Practical Chemistry, V K Alhuvalia, Sunita Dingra, 1 Edition, University Press, 2005
3. A collection of interesting general chemistry experiments, A. J. Elias, University Press, 2002
4. Inorganic Chemistry Practical, Deepak Pant, e-book, Book-Rix edition.
5. Lab Experiments in Organic Chemistry, Arunsethi, New Age International Publishers, 2010.
6. The Systematic Identification of Organic Compounds R.L. Shriner, C.K.F. Hermann, T.C. Morrill, D.Y. Curtin & R.C. Fuson John Wiley & Sons, Inc., 1997.
7. Identification of organic compounds. By N. D. Cheronis and J. B. Entrikin. Interscience Publishers, New York, 1963.
8. Organic Cum Practical Hand Book Of Organic Chemistry, B J Hassard
9. Organic Experiments, Louis F. Fisser, Kenneth Williamson, D.C. Heath and company, 1992.
10. A Hand Book Of Organic Analysis: Qualitative and Quantitative, Hans Thacher Clarke,1916.
11. Experimental Organic Chemistry, H Dubont Durst And George W Gokal, 2nd Edn., New York: McGraw Hill, 1987.
12. Practical Organic Chemistry, F G Mann and B C Saunders, 4th Edn., Pearson Education Ltd., 2009.
13. Textbook Of Practical Organic Chemistry, A I Vogel, Prentice Hall; 5th Edn., 1989.
14. Systematic Organic Chemistry, Modern Methods of Preparation and Estimation. By W.M. Cumming, I. Vance Hopper, and T. Sherlock Wheeler, London, 1923.

III SEMESTER			
C7	**INORGANIC CHEMISTRY - III**		**15PCHC31**
Hrs / Week: 5	**Hrs / Sem.: 75**	**Hrs / Unit: 15**	**Credit: 5**

UNIT I: ORGANOMETALLIC CHEMISTRY – I

Objective: *To have some idea about organo metallic chemistry*

Organo metallic compounds – preparation and properties of organo-metallic compounds of Be, Mg, Hg, Cd, Zn, B, Al, Ge, Sn and Pb. Carbon σ donors – metal alkyl and aryls – Synthesis, reactions – structure and bonding in metal alkyl and aryls.

Carbon π- donors, chain π–donor ligands – olefin, acetylene and allyl π systems – Synthesis – structure and bonding in olefins, Zeise's salt, acetylene and π-allyl complexes.

UNIT II: ORGANOMETALLIC CHEMISTRY – II

Objective: *to have some idea about organo-metallic chemistry*

Metallocenes: Synthesis and properties of Bessylocene molybdenocene, ferrocene, magnocenes -Structure and bonding of ferrocene.

Catalysis – hydrogenation of olefins (Wilkinson's catalyst), Hydroformylation of olefins using a Cobalt or Rh catalyst (oxo process), Oxidation of olefins to –CHO or –CO- (Wacker process), Polymerization (Ziegler'sNatta Catalyst), Cyclooligomerization of olefins and acetylenes using Ni catalyst (Reppe's catalyst).

UNIT III: BIOINORGANIC CHEMISTRY - I

Objective: *To understand the role of inorganic chemistry in enzymatic reactions*

Metalloproteins – structure and function of Hemoglobin, Myoglobin and Cytochrome – Binding of dioxygen and heme, myoglobin. Physiology of myoglobin and hemoglobin- Bohr Effect – Structure and function of Hemerythin, hemocyanine, Ferredoxins, Rubredoxins, Blue copper protein. Role of Mg in Photosynthesis

UNIT IV: BIOINORGANIC CHEMISTRY – II

Objective: *To study about the role of metals in bio-inorganic compounds*

Metal storage protein - Ferritin, transferrin and ceruloplasmin.

Iron storage and transport by siderphores, metal ion exchange activity of siderphores.

Structure and function of superoxide dismutase (SOD) – cytochrome oxidase – coenzymes. Molybdenum enzyme – Xanthine oxidase.

Zinc enzymes – carbonic anhydrase, carboxy peptidase and vitamin B_{12} coenzymes.

Sodium – potassium ion pump. Structure and Applications of cis- platin.

UNIT V: SPECTROSCOPY

Objective: *To have an idea about Mossbauer, NMR and EPR spectroscopy*

Mossbauer spectroscopy:

Principles – isomer shift, quadrupole and magnetic interactions – MB spectroscopy of octahedral high and low spins Fe(II) complexes. Information on oxidation state, pi-back coordination and structure in iron compounds. Studies on halides of tin (II) and tin (IV).

NMR:

Application of Chemical shift and spin-spin coupling to structure determination using multiprobe NMR (^{31}P, ^{19}F): effect of quadrupolar nuclei on NMR spectra. NMR studies on Chemical exchange and dynamic processes in inorganic and org anometallic compounds. NMR studies on fluxional molecules. Paramagnetic NMR and contact shifts: lanthanide shift reagents.

EPR:

Application of hyperfine splitting and g-factor to structure determination zero field splitting and Krammer's degeneracy, Covalence of M-L bonding and Jahn Teller distortion.

~~**ORGANOMETALLIC CHEMISTRY – III**~~

~~Transition metal – hydrogen compounds. General synthetic methods, Chemical behavior, characterization and H bridges, mononuclear polyhydrides, carbonyl hydrides and molecular hydrogen compounds. Transition metal carbon compounds, metal c single bond compounds and their reactions, alkylidyne complexes. Cyclometallation reactions~~

References:

1. Inorganic Chemistry - Principles, Structure and Reactivity, J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi,4th Edn., Pearson Education, 2006 .
2. Advanced Inorganic Chemistry, F. A. Cotton, G. Wilkinson, C.A. Murillo & M. Bochmann, 6th Edn., Wiley India Pvt. Ltd., 2014.
3. Bio-inorganic Chemistry, K. Hussain Reddy, 1st Edn., Newage Publishers, 2003.
4. Advanced Inorganic Chemistry, Satyaprakash, G.D. Tuli and S.K. Basu., Volume 1, S. Chand and Company, 2006
5. Modern Inorganic Chemistry, Willam L. Jooly, Magraw-Hill, 1991
6. Fundamentals of Molecular Spectroscopy, C. N. Banwell & E. M. McCash, Tata McGraw-Hill, New Delhi, 2006.
7. . Physical Methods in Chemistry, R. S. Drago, Saunders College Publishers, 1977.
8. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Horwood, New York, 1990.
9. NMR Spectroscopy in Inorganic Chemistry J. A. Iggo, Oxford University Press, Oxford, 2000

10. Mossbauer Spectroscopy, Greenwood, N. N. and T. C. Gibb, Chapmann and Hall, 1971.
11. Physical Methods for Chemists , Russell S. Drago , 2nd Edition, Surfside Scientific Publishers,1992.

III SEMESTER			
C8	**ORGANIC CHEMISTRY - III**		**15PCHC32**
Hrs / Week: 5	**Hrs / Sem.: 75**	**Hrs / Unit: 15**	**Credit: 5**

UNIT I: MOLECULAR REARRANGEMENT

Objective: *To have some idea about molecular rearrangement*

Rearrangement involving migration of electron deficient carbon – Pinacol – pinacolone rearrangement - Baeyer-Villiger Rearrangement – Wolff rearrangement – Benzil- Benzilic acid rearrangement.

Rearrangement involving migration of electron deficient nitrogen – Beckmann rearrangement – Lossen rearrangement - Schmidt rearrangement.

Rearrangement involving migration of electron deficient oxygen – Dakin reaction.

Rearrangement involving migration to electron rich carbon – Favorski rearrangement – Sommelet Hauser rearrangement.

Aromatic rearrangement – Hoffmann – Martius rearrangement

Rearrangement involving migration of oxygen to ring – Fries rearrangement – Sigmatropic rearrangement - Claisen rearrangement

~~**PERICYCLIC REACTIONS**~~

~~Dienophile, diene, Cyclic dienes, Heterodienes – Regiochemistry and Stereochemistry of the Diels-Alder reaction Intramolecular Diels-Alder reactions The retro Diels-Alder reaction – Asymmetric Diels-Alder reactions.~~

~~[2+2] Cycloaddition reactions - Cycloaddition reactions with allyl cations and allyl anions – 1,3 Dipolar cycloaddition reactions.~~

~~The ene reaction - [3,3]-Sigmatropic rearrangements – Cope rearrangement and Cope rearrangement – [2,3] Sigmatropic rearrangements - Electrocyclic reactions.~~

UNIT II: ORGANIC SPECTROSCOPY-I

Objective: *To have an idea about UV and IR spectroscopy*

Electronic spectra – Principle – selection rule- Rotational structure of electronic- vibration spectra – Franck Condon principle – types of electronic transitions – solvent effect – blue shift, red shift – Calculation of λ_{max} by Woodward Fieser rule and Scott rule – Applications of UV spectroscopy

Vibrational Spectra – Theoretical principle – Harmonic oscillator – anharmonicity – determination of force constant – Rotational – Vibrational spectra of diatomic molecules, - P,Q,R branches – Vibrational spectra of polyatomic molecules – normal modes of vibration of CO_2, H_2O. Vibrational frequencies – Factors affecting IR

spectra – Finger print region – Fermi resonance – Applications of IR spectroscopy.

~~ALKALOIDS~~

~~Occurrence, Classification, Structural elucidation and synthesis of quinine, nicotine, morphine, lysergic acid and reserpine.~~
~~Biogenesis of alkaloids~~

UNIT III: ORGANIC SPECTROSCOPY-II

Objective: *To have an idea about NMR spectroscopy*

^{1}H-NMR spectroscopy – principle – relaxation effect, chemical shift, factors influencing chemical shift – spin-spin coupling constant – PMR spectrum of simple molecules- 1-propanol, 1,1,2-tribromoethane, ethyl acetate, benzaldehyde, acetaldehyde, ethyl methyl ketone, isopropyl alcohol – ^{13}C NMR Principle.

Multidimensional NMR Spectroscopy: From 1-D to 2-D to n-D – homonuclear coherence transfer and mixing: COSY, DEPT, NOESY, TOCSY.

~~STEROIDS & TERPENOIDS~~

~~Steroids: Structural elucidation of cholesterol Occurrence – Synthesis and structure (only) of Ergosterol, Testosterone, Oestrone, Oestriol, Equilinin and Progesterone – Bile acids Prostaglandins – structure and synthesis of PGE_1 and PGF_1.~~

~~Terpenoids: Classification – Isoprene rule, calculation of λ_{max}, Structural elucidation of citral, camphor α-pinene, zingiberne and abietic acid.~~

UNIT IV: ORGANIC SPECTROSCOPY-III

Objective: *To have an idea about Mass spectrometry*

Mass spectrometry – Principle – Instrumentation – m/e, m/z, fragmentation pattern, Types of ions, Nitrogen rule, Mclafferty rearrangement - Relative abundance of isotopes, chemical ionization, Various types of Mass spectrometry - FABMS, EIMS, MALDI, MALDITFR, ICPMS, HRMS.

~~VITAMINS~~

~~Vitamins-Types- Fat soluble, Water soluble, Structure (only) of vitamins A, B1, B_2, B_3, B_6, H. Structural elucidation of vitamins A, nicotinic acid, B_6 and H, Biosynthesis of vitamin C, vitamin P, antivitamins.~~

UNIT V: PERICYCLIC REACTIONS:

Objectives*: To have some elementary idea about pericyclic reactions*

Dienophile, diene, Cyclic dienes, Heterodienes - Regiochemistry and Stereochemistry of the Diels–Alder reaction-Intramolecular Diels–Alder reactions- The retro Diels–Alder reaction - Asymmetric Diels–Alder reactions.

[2+2] Cycloaddition reactions - Cycloaddition reactions with allyl cations and allyl anions - 1,3-Dipolar cycloaddition reactions.

The ene reaction - [3,3]-Sigmatropic rearrangements – C,ope rearrangement and Cope rearrangement - [2,3]-Sigmatropic rearrangements - Electrocyclic reactions.

~~ORGANIC SYNTHESIS~~

~~Disconnection approach: An introduction to synthesis, and synthetic equivalents, functional group inter-conversions, disconnection, synthon, Retrosynthesis, Importance of the order of events in organic synthesis – one group C-X disconnections- acid derivatives and alcohols, chemoselectivity.~~

~~Reversal of polarity – cyclisation reactions.~~

~~Disconnection Analysis Butylated hydroxy toluene, Piperonal, Trifluralin B.~~

REFERENCES

1. Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, J. March, M.B. Smith, 6th Edn., Wiley, 2007.
2. Advanced Organic Chemistry, Part B: Reactions and Synthesis, F.A. Carey, R.A. Sundberg, 5th Edn., Springer, 2007.
3. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.
4. Modern Methods of Organic Synthesis, W. Carruthers, I. Coldham, Cambridge University Press, 2005.
5. S. Sankararaman, Pericyclic Reactions-A Text Book, Wiley VCH, 2005.
6. Organic Chemistry, J. Clayden, N. Greeves, S. Warren, P. Wothers, Oxford University Press, 2004.
7. Fundamentals of Photochemistry – K. K. Rohatgi – Mukherjee (Revised Edition) New age International publications, Reprint 2002.
8. Photochemistry in Organic Synthesis, J.D. Coyle – Royal society of Chemistry, 1986.
9. Organic Chemistry, Volume II, Stereochemistry and the Chemistry of Natural Products, I.L. Finar, Longmans, 1964.

III SEMESTER			
C9	**PHYSICAL CHEMISTRY - III**		**15PCHC33**
Hrs / Week: 5	**Hrs / Sem.: 75**	**Hrs / Unit: 15**	**Credit: 5**

UNIT I: STATISTICAL MECHANICS-I

***Objectives**: To know the fundamental of statistical mechanics.*

Degrees of freedom – translational, rotational and vibrational degrees of freedom – Phase space - Unit cells – Microstate – Macrostate – systems (open, closed, isolated) – Assembly – Ensembles - types of ensembles - ensemble average – Statistical equilibrium. Thermodynamic probability – Stirling's theorem

~~**PHOTOCHEMISTRY**~~

~~Physical properties of electronically excited molecules – excited state dipole moment – excited state redox potentials – photo physical processes in electronically excited molecules – fluorescence, phosphorescence, internal conversion, intersystem crossing – delayed fluorescence, P – type and E – type – Stern – Volmer equation and its applications – experimental techniques in photochemistry – chemical actinometry and flash photolysis Elementary aspects of photosynthesis~~.

UNIT II: STATISTICAL MECHANICS-II

***Objectives**: To know the fundamental of statistical mechanics.*

Molecular Basis of residual entropy – Boltzmann distribution law-comparison – Partition function – Evaluation of Translational, Rotational, Vibrational and Electronic partition function –Relation between partition function and Enthalpy, C_v, C_p, Entropy, Helmholtz free energy, Pressure, Gibb's free energy, enthalpy and chemical potential – Thermodynamic properties of an ideal monoatomic and diatomic gas.

~~**STATISTICAL THERMODYNAMICS-I**~~

~~Modern Theoretical principals: Exact and inexact differential expressions in two variables – Total differentials – Techniques of partial differentiations – Transformation of variables - Maxima and mimima – Integrating factors, Paff differential equations, Caratheodorys theory – Legendre transformations – Derivation of thermodynamic identities – The second law of thermodynamics, classical formulations, mathematical consequences of second law – Entropy changes , Clausius inequality – Free energy concept – General condition of equilibrium – Thermodynamic potentials.~~

UNIT III: GROUP THEORY – I

***Objective**: To have an idea about Group theory*

Group theory – Symmetry elements – symmetry operations – Postulates of Group-Point groups – C_p, C_{2v}, C_{3v}, C_{2h}, D_2, D_6, D_{2d}, D_{2h} – Determination of Point groups – Representation of molecular point

groups – reducible representation and irreducible representation– Great orthoganality theorem (GOT) – Use of GOT to construct character tables – character tables for point groups – C_{2v}, C_{3v},C_{2h},D_{3h}

~~STATISTICAL THERMODYNAMICS-II~~

~~Phase space, stirlings approximation, Configuration and weights, the most probable configuration - Statistical Equilibrium - Postulates of equal probabilities – Ensembles – Ensemble average and time average of property – The Boltzmann Distribution law – Principle of the equipartition of energy , Quantum Statistics : BE and FD statistics, comparison of three statistics and radiation , Fermi – Dirac systems. Fermy energy – Electron gas in metals.~~

UNIT IV: GROUP THEORY – II

Objective: *To have an idea about the applications of Group theory*

Reducible representation into its irreducible representation- Rules for determining the irreducible representation of Vibrational modes-normal modes of vibration of polyatomic molecules-H_2O-NH_3,BF_3-Direct product of irreducible representation- selection rule for the π-π^*& π-π^* transition in HCHO construction of Hybrid orbitals-CH_4, $[PtCl_4]^{2-}$–secular equation in MO theory-trans 1,3-butadiene, Benzene.

~~QUANTUM CHEMISTRY– III~~

~~Hydrogen atom – Radial distribution function – Angular part of the wave function – Electron spin – Quantum numbers-~~

~~Wave function of many electron systems – Helium atom – Pauli's exclusion principle – Slater determinants – Angular Momentum – Commutators relations – step up and step down operators – angular momentum in many electron atom – Spin – orbit interaction.~~

UNIT V : CHEMICAL KINETICS – II

Objectives*: To know about the kinetics of different reaction*

Oscillatory reactions – Belousov Zhabotinskii reaction – Kinetics of solid state reactions – Kinetics of reaction in solution – Debye Ryduchowski reaction – Influence of ionic strength (salt effect). Influence of solvent on reaction rate – Secondary salt effect – Kinetic isotopic effect – solvent isotope effect – Hammett equation – linear free energy relationship – Taft equation – Compensation effect.

Kinetics of fast reaction – Flow methods for fast reaction – stopped flow method – quenched flow method – Relaxation method – Pulse radiolysis – flash photolysis.

~~QUANTUM CHEMISTRY– IV~~

~~General time - independent perturbation theory – Applications to hydrogen and Helium atoms - Variation theorem – Application to hydrogen and helium atoms – Time dependent perturbation theory- Born-Oppenheimer approximation –MO theory - LCAO approximation – MO method for H_2^+ and H_2 – VB treatment of H_2 molecule – Excited state of Hydrogen molecule – Comparison of MO and VB theories~~

REFERENCES:

1. Quantum Chemistry, Donald A. Mcquire, Viva Books, 2011.
2. Quantum Chemistry, A.B. Samigrahi, Books and Allied Pvt. Ltd, 2010.
3. Introductory Quantum Chemistry, A.K. Chandra, 4th Edn., Tata McGraw Hill, 2001.
4. Quantum Chemistry, Ira N. Levin, Edition VI, PHI Learning PVT Ltd., New Delhi, 2009.
5. Molecular Quantum Mechanics, Atkins P W and R S Friedman, 3rd Edn., Oxford University Press,1996.
6. Molecular Modeling, Principles and Applications, Second Edition, Andrew R Leech, Prentice Hall, NY, 2001.
7. Guide Book on molecular modeling in Drug Design, N. Claude Cohen, 1st Edn.,, Academic Press, 1996.
8. Principles of Physical Chemistry, Puri, Sharma and Pathania, Vishal Publications, 2008.
9. Principles and Applications of Electrochemistry, Crow, D.R., Chapman and Hall, 1988.
10. Electrochemistry, Reiger, P.H., Chapman and Hall, 2nd Edn., 1983.
11. A.G. Marshall, Biophysical Chemistry, John Wiley and Sons, New York, 1978.
12. K.J. Laidler, Physical Chemistry with Biological Applications, Benjamin, 1980.

III SEMESTER Non-Major elective			
NME	CHEMINFORMATICS		15PCHN31A
Hrs / Week: 6	Hrs / Sem.: 90	Hrs / Unit: 18	Credit: 3

UNIT I: COMPUTER REPRESENTATION AND MANIPULATION OF 2D MOLECULAR STRUCTURE

Objective: *To know the basic idea about bioinformatics and databases*

Scope of Cheminformatics Computer - Representations of Chemical Structures, Graph Theoretic Representations of Chemical Structures, Connection Tables and Linear Notations, Canonical Representations of Molecular Structures - Structure Searching- Screening Methods, Algorithms for Subgraph Isomorphism, Practical Aspects of Structure Searching.

UNIT II: INTRODUCTION TO DATABASES & ITS CLASSIFICATION

Objective: *To know the basic idea about bioinformatics and databases*

Characteristics and categories of databases – Sequence databases – Nucleotide sequence databases – EMBL, DDBJ, GenBank – Secondary nucleotide sequence databases – UniGene, STACK, Ribosomal databases, HIV sequence database, REBASE – Protein sequence databases – UniProtKB, SWISSPROT, TremBL, PDB.

UNIT – III : DATABASES AND DATA SOURCES IN CHEMISTRY

Objective : *To know about the various database available for chemistry*

Classification of databases – Literature databases – Chemical Abstracts System (CAS) – SCISEARCH & MEDLINE – Factual databases – property databases – Beilstein and Gmelin – Crystal structure databases – CSD, ICSD– Structure databases - NCI – Chemical reaction databases – Classification of Scientific Literature - primary, secondary and tertiary literature – Online databases – access to CAS with SciFinder Scholar 2002.

UNIT –IV: CHEMICAL INFORMATION SEARCHES & STRUCTURE DESCRIPTORS

Objective : *To study about the chemicals information searches and structure descriptors*

Full structure search – Substructure search – Backtracking algorithm- Screening – similarity search –similarity measure – Tanimato – 3D structure search.

Descriptors Definition – classification – structure keys – topological description – 3 D descriptors – chirality descriptors – Conformation independent and conformation dependent.

UNIT V: APPLICATIONS OF CHEMINFORMATICS

Objective: *To have an idea about the applications of cheminformatics.*

Prediction of properties – estimation of log Pw, log S & Toxicity- prediction of spectral properties – chemical shift, IR simulation and mass spectra - prediction of chemical reactions – computer assisted synthesis design – Drug design – target identification & validation – lead finding and optimization – design of combinatorial libraries – Structure based and ligand based drug design

REFRENCES:

1. Computational Molecular Biology, Pevzner, P.A, Prentice Hall of India Ltd, New Delhi, 2004.
2. Bioinformatics and Functional Genomics, Pevsner, J., John Wiley and Sons, New Jersey, USA, 2003.
3. Bioinformatics: Sequence and Genome Analysis, Mount, D), Cold Spring Harbor Laboratory Press, New York, 2004.
4. Bioinformatics – a practical guide to the analysis of Genes and Proteins, Baxevanis, A.D. and Francis Ouellellette, B.F.(), John Wiley & Sons, UK, 1998.
5. Molecular Modeling, Principles and Applications, II Edition, Andrew R. Leach, Dorset Press, Dorchester, Dorset, 2001.
6. Cheminformatics, ed., Johann Gasteiger and Thomas Engel, Wiley VCH, Weineim, 2003.
7. Introduction to Chemiformatics, Andrew.R. Leach and Valeric J Gillet, Springer, 2007.

III SEMESTER			
DSE3A	INSTRUMENTAL METHODS OF ANALYSIS		18PECH3A
Hrs / Week: 4	Hrs / Sem.: 60	Hrs / Unit: 12	Credit: 4

UNIT I - THERMOANALYTICAL METHODS

Thermo Gravimetric Analysis (TGA) – principle, instrumentation, application – Factors affecting TGA Differential Thermal Analysis (DTA) – principle and instrumentation, DTA of Calcium oxalate monohydrate – Comparison of DTA - TGA curves.

UNIT – II - ELECTRO-ANALYTICAL METHODS

Electro Gravimetric Analysis (EGA) – theory, types of EGA, instrumentation and applications in the estimation of metal ions in solution. Polarography – principle – dropping mercury electrode (DME). Advantages of DME- applications

UNIT III: COLORIMETRIC, SPECTROPHOTOMETRIC ANALYSIS , IR & RAMAN SPECTROSCOPY

Visible colorimetry – Principle, instrumentation –Applications. Spectrophotometer instrumentation Applications UV VIS Spectrophotometer – Single beam and Double – beam Spectrometer - Applications – IR spectrometer theory, principle, instrumentation sampling techniques- factors influencing vibrational frequencies Applications. Raman spectroscopy Raman Effect Conditions for Raman spectrum, Instrumentation – Comparison between IR and Raman Spectroscopy.

UNIT IV: FLUOROMETRY, FLAME AND NEPHLOMETRY ANALYSIS

Fluorometry – principle – instrumentation and applications. Flame photometry – principle – instrumentation and applications. Nephelometry and turbidimetry - theory - instrumentation and applications. Atomic Absorption Spectroscopy Principle, Instrumentation Spectral and Chemical Interferences Applications.

UNIT V: NMR, PHOTOELECTRON SPECTROSCOPY AND MEDICAL IMAGING TECHNIQUES

NMR spectroscopy, Principle and Instrumentation. Applications. Photoelectron Spectroscopy – principle – Instrumentation. Medical Imaging- Magnetic Resonance Imaging (MRI) **Positron emission tomography** (PET) , **Single-photon emission computed tomography** (**SPECT**). **Computer-assisted tomography (CT)** , Echocardiography Basic theory and Applications

REFERENCES:

1. Fundamentals of Analytical Chemistry – D.A.Skoog, D.M. West, F.J. Holler and S.R. Crouch – 2004; Thompson Asia Private Ltd., Bangalore.
2. Instrumental Methods of Analysis – B. K. Sharma, 2003; Goel publishing House, Meerut.

3. Contemporary Chemical Analysis – Judith F. Rubinson, Prentice Hall (India).
4. Instrumental Methods of Analysis Hobart H. Willard, Lynne L. Merritt Jr, John Dean, Wadsworth Publishing Co Inc; 7th Edn., 1988.
5. Thin Layer Chromatography- A laboratory Handbook, Ashworth, Stahl. E., 1st Edn., Springer Verlag, 1969.
6. Dynamics of Chromatography – Principles and Theory, J. Calvin Giddings, CRC Press, 2002.
7. Spectroscopy of organic compounds, Kalsi, P.S., New Age Publishers New Delhi, 2007.
8. Principles of Instrumental Analysis, Douglas A. Skoog, F. James Holler, Stanley R. Crouch, 2006.
9. Fundamentals of Medical Imaging, Paul Suetens, 2nd Edition, Cambridge University Press, 2002.

III SEMESTER Non-Major elective			
NME	**APPLIED CHEMISTRY**		**15PCHN31B**
Hrs / Week: 6	**Hrs / Sem.: 90**	**Hrs / Unit: 18**	**Credit: 3**

UNIT I- PETROLEUM AND PETROCHEMICALS

Objective: *To study the importance of petroleum and petrochemicals.*

Refining of petroleum – Composition and uses of main petroleum fractions – Cracking – Thermal and catalytic cracking – Types of catalytic cracking Advantages of catalytic cracking – Octane number – Antiknock agents – Unleaded petrol – Cetane number – Anti diesel knock agents – Flash point – synthetic petrol – Fischer Tropsch process. Petrochemicals – manufacture and industrial uses of methanol – ethanol – rectified sprit, methylated sprit, absolute alcohol – Industrial uses of isopropanol, ethylene glycol, glycerin, acetone and phenol.

UNIT II - PLANT NUTRIENTS / FERTILIZERS

Objective: *To understand the idea about the plant nutrients/fertilizers and their importance.*

Plant nutrients – Macro and micro nutrients – Their role in plant growth – Sources, forms of nutrients absorbed by plants. Deficiency symptoms in plants – Corrective measures – Chemicals used for correcting nutritional deficiencies.

Fertilizers – Manures – Characteristics and its importance – Synthetic fertilizers – Manufacture and uses of urea and Triplesuperphosphate, superphosphate of lime, CAN, Potassium nitrite, – Mixed fertilizers – Biofertilizers – Estimation of N by Kjeldhal method – Estimation of P by Olsen method. Estimation of K by flame photometer.

UNIT III- Industrial Chemistry

Objective: *To know the idea about paper, textile, match Industries and explosives.*

Chemistry of paper industry: Raw materials – manufacturing process – bleaching and colouring.

Textile Chemistry: Fibers – definition – natural and synthetic fibers – distinction – manufacture and uses of rayon, nylon 6-6, dacron, orlon and Teflon.

Match industry: Safety matches – composition of the match head, composition of fireworks – coloured matches Pyrotechnic and Explosives.

Explosives: classifications – primary explosives – preparation of lead azide, DDNP, Tetryl and EDNA. High explosives – Preparation of TNT, picric acid, Ammonium picrate, GTN, PETN, Cyclonite.

UNIT IV- PHARMACEUTICAL CHEMISTRY

Objective: *To study the structure and uses of the following important drugs.*

Structure and uses:

1) Sulpha drugs-sulphadiazine, protosil and prontosil
2) Antimalarials –quinine, plasmoquine
3) Arsenical drugs – Salvarasan 606, Neosalvarasan
4) Antibiotics - Penicillin, Tetracycline, Streptomycin and Chloromycin (structure and uses)

Anaesthetics – General anaesthetics- vinyl ether-cyclopropane-Halohydrocarbon-chloroform-Haloethane-Trichloro ethylene – Intravenous anesthetics-Thiopentone-sodium isoprenoid- Local anesthetics – Cocaine and its derivatives.

Preparation and uses of the following compounds:

Antacids – Magnesium trisilicate, Milk of magnesia
Antifungals - Griseofulvin
Emetic - Tartaremetic
Haematonics – Ferrous gluconate
Analgesic and Anripyretic – Aspirin.
Cancer – causes.

UNIT V- THERMO-ANALYTICAL AND ELECTRO-ANALYTICAL METHODS

Objective: *To study the analytical uses of thermal and electro analytical methods*

Thermo Gravimetric Analysis (TGA) – principle, application in the determination of optimum drying temperature range of the precipitates - Factors affecting TGA -Differential Thermal Analysis (DTA) – principle and instrumentation, DTA of Calcium oxalate monohydrate – Simultaneous DTA - TGA curves – Thermometric titration.

Electro Gravimetric Analysis (EGA) – theory, types of EGA; instrumentation and applications in the estimation of metal ions in solution. Polarography – principle – dropping mercury electrode (DME) – Amperometric titration.

REFERENCE BOOKS:

1. Industrial Chemistry – B.K.Sharma, 2003, Goel Publishing House, Meerut.
2. Industrial Chemicals – Faith etal, Wiley Interscience, New York.
3. Chemical Process Industries - R.N. Shreve, 2000; Tata McGraw Hill Publishing Company, Mumbai.
4. Text Book of Pharmaceutical Chemistry – Jaysgree Ghosh, 2003; S. Chand and Company, New Delhi.
5. Fundamentals of Analytical Chemistry – D.A.Skoog, D.M. West, F.J. Holler and S.R. Crouch – 2004; Thompson Asia Private Ltd., Bangalore.

III SEMESTER			
DSE3B	ENZYME CHEMISTRY		18PECH3B
Hrs / Week: 4	Hrs / Sem.: 60	Hrs / Unit: 12	Credit: 4

UNIT I: ENZYME - INTRODUCTION

Enzyme Classification and nomenclature – isolation and purification properties of enzymes – enzyme specificity effect of pH, temperature, concentration of enzyme, concentration of substrate on enzyme activity and stability – units of enzyme activity and stability – co-enzymes and co-factors.

UNIT II: KINETICS AND MECHANISM OF ENZYME CATALYZED REACTION

Induced fit reaction – Lock and key mechanism – Kinetics and mechanism of enzyme catalysed reaction – Steady state kinetics – Derivation of Michealis Menton equation – significance of V_{max} and k_m – L plot – Multistage enzyme kinetics – pre steady state relaxation kinetics – King and Allman procedure – Negative and positive cooperativity (feedback inhibition) – enzyme inhibition – enzyme immobilization and its application.

UNIT III: MECHANISM OF ENZYMES AND TYPES

Active sites – Mechanism of enzyme action – lysoyme, chymotrypsin, DNA polymerase RNAse, isoenzymes (lDH), allosteric enzyme, ribozyme & abzyme.

UNIT IV: MULTI ENZYME COMPLEX

Multienzyme complexes – structure and function of pyruvate dehydrogenase and fatty acid synthase complex – Advantages of multienzyme complex – Commercial application of enzymes in food pharmaceutical and other industries – enzymes for diagnostic applications – Biosenors

UNIT V: EXTREMOZYMES

Extremozymes – Extremophiles – Thermophiles – Halophiles – Psychrophiles – Industrial application – protein engineering (site – directed mutagenesis).

REFERENCES

1. Biochemistry, Lehinger, J., CBS. Publishers, 1993
2. Biochemistry, D.Voet and JG, Voet, John Wiley & Sons, Inc. 2nd Edn., 1995.
3. Fundamentals of Biochemistry, Jain J.L Chand & Co, New Delhi, 2000
4. Biochemistry, Davison, V.L. & Sitlmon, D.L. 4th Ed, Lippinocoth William & Willeing, 1999

Enzymolgy, Malcom Dixon and Edwin C. Webb Academic Press, 2nd Ed. edition 1964

Enzyme Technology, Martin Chaplin, Christopher Bucke, Cambridge University Press, 1990

~~Enzyme Technology, Ashok Pandey, Colin Webb, Carlos Ricardo Soccol, Christian Larroche, Asiatech Publishers Inc., 2005~~
~~Enzyme Technology, S. Shanmugham, I. K. International Pvt. Ltd., 2009~~
~~Enzymology and Enzyme Technology, S.M. Bhatt, S. Chand, 2011~~
~~Enzyme Technology, Anusha Bhaskar, V.G. Vidhya, MJP Publishers, 2009~~

III SEMESTER		
P V	ORGANIC CHEMISTRY PRACTICAL – II	18PCCH3P1
Hrs / Week: 4	Hrs / Sem.: 60	Credit: 2

I. Estimation of Organic Compounds

1. Estimation of Glucose by Bertrand's method.
2. Estimation of Glucose by Lane-Eynon's method
3. Estimation of Ethyl Methyl Ketone
4. Estimation of an Amino group [By Bromination reaction]
5. Estimation of Iodine value of oil(Course work)

II Preparation of Organic Compounds [Double Stage preparations]

1. Preparation of *p*- Bromo aniline from Acetanilide
2. Preparation of *p*- Nitroaniline from Acetanilide
3. Preparation of 2,4,6-Tribromobenzene from Aniline
4. Preparation of Benzanilide from Benzophenone
5. Preparation of Phthalamide from Phthalic acid
6. Preparation of *m*-Nitrobenzoic acid from *m*-Nitrobenzoate
7. Preparation of Benzilquinoxaline from Benzoin
8. Preparation of *p*-Aminobenzoic acid from *p*-Nitro Toluene
9. Preparation of Caprolactum from Cyclohexanone(Course work)

REFERENCES:

1. Lab Experiments in Organic Chemistry, Arunsethi, New Age International Publishers, 2010.
2. The Systematic Identification of Organic Compounds R.L. Shriner, C.K.F. Hermann, T.C. Morrill, D.Y. Curtin & R.C. Fuson John Wiley & Sons, Inc., 1997.
3. College Practical Chemistry, V. K. Ahluwalia, Sunita Dhingra and Adarsh Gulati, by University Press, Hyderabad, 2012.
4. Identification of Organic Compounds. By N. D. Cheronis and J. B. Entrikin. Interscience Publishers, New York, 1963.
5. Organic Experiments, Louis F. Fisser, Kenneth Williamson, D.C. Heath and company, 1992.
6. Experimental Organic Chemistry, H Dubont Durst and George W Gokal, 2nd Edn., New York: McGraw Hill, 1987.
7. Practical Organic Chemistry, F G Mann and B C Saunders, 4th Edn., Pearson Education Ltd., 2009.
8. Textbook Of Practical Organic Chemistry, A I Vogel, Prentice Hall; 5th Edn., 1989.
9. Systematic Organic Chemistry, Modern Methods of Preparation and Estimation. By W.M. Cumming, I. Vance Hopper, and T. Sherlock Wheeler, London, 1923.

III SEMESTER		
P-VI	PHYSICAL CHEMISTRY PRACTICAL II	18PCCH3P2
Hrs / Week: 4	Hrs / Sem.: 60	Credit: 2

1. Verification of Ostwald's dilution law
2. Primary salt effect (Course Work)
3. Kinetics of persulphate – iodide reaction in solution
4. Study of distribution of benzoic acid
5. Comparison of acid strength by ester hydrolysis
6. Determination of heat of solution of naphthalene – toluene system
7. Determination of heat of solution of oxalic acid – water system
8. Determination of heat of solution of ammonium oxalate – water system
9. Adsorption of acetic acid / oxalic acid on activated charcoal – verification of Freundlich isotherm determination of unknown concentration
10. Determination of partial molar volume of solute (eg. KCl) and solvent in a binary mixture.
11. Determination of stoichiometry and stability constant of inorganic and organic complexes.
12. Computational Chemistry (course work)

Draw the structure of simple molecules (CH_4 / Ethane / Water/ toluene/ benzene/ HCHO) in:

- Gauss View
- Chem3D

Observe the amount of effort required in each case.

Use GaussView version of the above molecules as .mol file and read it with Gaussian.
Run geometry optimizations using
a. Hartree-Fock (HF / STO-3G)
b. HF / 3-21G
c. HF / 6-31G*
Observe the time taken for running each molecule. Save the output file.

Read the .mol file with Gauss View and set up a Gaussian job for the above molecules and run geometry optimization using DFT with B3LYP / 6-31G* (reasonable accuracy) basis set. Save the output file.

REFERENCES:

1. Experimental Physical Chemistry: A Laboratory Textbook, Arthur Halpern, George McBane, 2006.
2. A Manual of Practical Physical Chemistry, Francis William Gray, 2010.
3. Physical Chemistry Laboratory Manual, Robb J. Wilson, 2010.
4. Practical Physical Chemistry, Alexander Findlay, 2012.

5. Physical Chemistry Laboratory, L. Peter Gold, McGraw Hill PVT Ltd., 1997.
6. www.gaussian.com

IV SEMESTER			
C10	ORGANIC CHEMISTRY - IV		15PCHC41
Hrs / Week: 5	Hrs / Sem.: 75	Hrs / Unit: 15	Credit: 5

UNIT I: STEROIDS

Objectives: *To have an idea about steroids*

Occurrence- classification – reactions, structural elucidation of cholesterol – Synthesis and structure of Ergosterol, Testosterone, Oestrone, Oestriol, Equilinin and Progesterone – Bile acids- Prostaglandins - general study - structure and synthesis of PGE_1 and PGF_1.

UNIT II: VITAMINS

Objectives: To know about the structure and functions of vitamins

Sources, structure and functions of retinol, thiamine, riboflavin, pyridoxine, cyanocobalamin, ascorbic acid, ergocalciferol, tocopherols and K_1. Synthesis of vitamin B_2, vitamin B_{12} vitamin D and biotin.

Unit III: ORGANIC SYNTHESIS - I

Objectives: *To understand the protection and disconnection approaches applied in organic synthesis*

Protection of groups: Principle of protection of hydroxyl, amino, carbonyl, carboxylic acid with different reagents and their deprotection, synthetic equivalent groups, synthetic analysis and planning, control of stereochemistry.

Disconnection approach: An introduction to synthesis, and synthetic equivalents, disconnection approach, functional group inter-conversions, importance of the order of events in organic synthesis one group C-X and two group C-X disconnections, chemoselectivity, reversal and polarity.

Unit IV: ORGANIC SYNTHESIS - II

Objectives: *To understand the protection and disconnection approaches applied in organic synthesis*

One group C-C disconnections -Alcohols and carbonyl compounds, regio-selectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

Disconnection Analysis- Butylated hydroxy toluene, Piperonal, Trifluralin B, Saccharine

UNIT V: BIOSYNTHESIS OF ORGANIC COMPOUNDS

***Objectives**: To understand the biosynthesis of some natural products*

Biosynthesis of cholesterol, α- terpineol, morphine.

Biogenesis of alkaloids.

Reference books:

1. Chemistry of Natural Products, S.V. Bhat, B.A. Nagasampagi, N. Sivakumar, Narosa Publishing House, New Delhi, 2010.
2. Organic Chemistry, I L Finar, Vol II ELBS, 5th Edn., 2000
3. Medicinal Chemsitry, Ashutosh Kar, 2nd Edn., New Age International (Pvt.) Publishers, 2007.
4. Organic Chemistry of Natural Products, Volume II, Chatwal Gurdeep R, Himalaya Publishing House, 2009.
5. Organic synthesis: The Disconnection Approach, Stuart Warren and Paul Wyatt, 1st Edition, Wiley student edition, 1982
6. Workbook for Organic Synthesis: The Disconnection Approach" by Stuart G. Warren, Wiley, 1983.
7. Fundamentals of Medicinal Chemistry, Gareth Thomas, John Wiley & Sons Ltd., 2003.
8. Combinatorial Chemistry Synthesis and Application, Stephen R. Wilson, Anthony W. Czarnik, Wiley, 1997.
9. Biomimetic Organic Synthesis, Erwan Poupon, Bastien Nay, Wiley-VCH, Verlag, Germany, 2011.
10. Biosynthesis, Volume 5, J. D. Bu'Lock, Royal Society of Chemistry, 1977.

~~IV SEMESTER~~			
~~DSC10~~	~~SPECTROSCOPY~~		~~18PCCH41~~
~~Hrs / Week: 5~~	~~Hrs / Sem.: 75~~	~~Hrs / Unit: 15~~	~~Credit:4~~

~~UNIT I: ORGANIC SPECTROSCOPY-I~~

~~**Electronic spectra** – Principle – selection rule Rotational structure of electronic- vibration spectra – Franck Condon principle – types of electronic transitions – solvent effect – blue shift, red shift – Calculation of λ_{max} by Woodward Fieser rule and Scott rule – Applications of UV spectroscopy~~

~~**Vibrational Spectra** – Theoretical principle – Harmonic oscillator – anharmonicity – determination of force constant – Rotational – Vibrational spectra of diatomic molecules, P,Q,R branches – Vibrational spectra of polyatomic molecules – normal modes of vibration of CO_2, H_2O. Vibrational frequencies – Factors~~

affecting IR spectra – Finger print region – Fermi resonance – Applications of IR spectroscopy.

UNIT II: ORGANIC SPECTROSCOPY-II

^{1}H NMR spectroscopy – principle – relaxation effect, chemical shift, factors influencing chemical shift – spin spin coupling constant – PMR spectrum of simple molecules – 1 propanol, 1,1,2 tribromoethane, ethyl acetate, benzaldehyde, acetaldehyde, ethyl methyl ketone, isopropyl alcohol – ^{13}C NMR Principle.

Multidimensional NMR Spectroscopy: From 1 D to 2 D to n D – homonuclear coherence transfer and mixing: COSY, DEPT, NOESY, TOCSY.

UNIT III: ORGANIC SPECTROSCOPY-III

Mass spectrometry – Principle – Instrumentation – m/e, m/z, fragmentation pattern, Types of ions, Nitrogen rule, Mclafferty rearrangement – Relative abundance of isotopes, chemical ionization, Various types of Mass spectrometry – FABMS, EIMS, MALDI, MALDITFR, ICPMS, HRMS.

UNIT IV: ORD, CD

Principle – types of ORD curves – axial haloketone rule – octant rule – applications of these in the determination of configuration and conformation of simple monocyclic and bicyclic ketones.

UNIT V: INORGANIC SPECTROSCOPY

Mössbauer speetroscopy:

Principles – isomer shift, quadrupole and magnetic interactions – MB spectroscopy of octahedral high and low spins Fe(II) complexes. Information on oxidation state, pi back coordination and structure in iron compounds. Studies on halides of tin (II) and tin (IV).

NMR:

Application of Chemical shift and spin-spin coupling to structure determination using multiprobe NMR (^{31}P, ^{19}F): effect of quadrupolar nuclei on NMR spectra. NMR studies on Chemical exchange and dynamic processes in inorganic and org anometallic compounds. NMR studies on fluxional molecules. Paramagnetic NMR and contact shifts: lanthanide shift reagents.

EPR:

Application of hyperfine splitting and g factor to structure determination zero field splitting and Krammer's degeneracy, Covalence of M-L bonding and Jahn Teller distortion.

REFERENCES

1. Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, J. March, M.B. Smith, 6th Edn., Wiley, 2007.
2. Advanced Organic Chemistry, Part B: Reactions and Synthesis, F.A. Carey, R.A. Sundberg, 5th Edn., Springer, 2007.
3. Advanced Organic Chemistry: Reaction Mechanism, R. Bruckner, Academic Press, 2002.
4. Modern Methods of Organic Synthesis, W. Carruthers, I. Coldham, Cambridge University Press, 2005.

5. Pericyclic Reactions A Text Book, S. Sankararaman, Wiley VCH, 2005.
6. Organic Chemistry, J. Clayden, N. Greeves, S. Warren, P. Wothers, Oxford University Press, 2004.
7. Organic Chemistry, Volume II, Stereochemistry and the Chemistry of Natural Products, I.L. Finar, Longmans, 1964.

IV SEMESTER			
C11	PHYSICAL CHEMISTRY – IV		15PCHC42
Hrs / Week: 5	Hrs / Sem.: 75	Hrs / Unit: 15	Credit: 5

UNIT I: QUANTUM CHEMSITRY IV

Objective: *To have an idea about quantum chemistry*

– General time –independent perturbation theory – Applications to hydrogen and Helium atoms - Variation theorem – Application to hydrogen and helium atoms – Time dependent perturbation theory- Born-Oppenheimer approximation –MO theory - LCAO approximation – MO method for H_2^+ and H_2 – VB treatment of H_2 molecule – Excited state of Hydrogen molecule – Comparison of MO and VB theories

UNIT II: QUANTUM CHEMSITRY V

Objective: *To have an idea about theories in quantum chemistry*

Hybridization – solving wave functions for sp, sp^2, sp^3 hybrid orbitals,- Huckel molecular Orbital theory for the linear conjugated system - HMO theory of ethylene, butadiene and benzene –Calculation of bond order and charge density calculation. Self-consistent- field approximation – Hartree's theory - Hartree-Fock SCF theory – Koopmann theorem

UNIT III: QUANTUM CHEMSITRY VI

Objective: *To have an idea about theories and methods in quantum chemistry*

Semi-empirical SCF theory – Basis sets – Slater type orbitals and Gaussian type orbitals – Classification of basis sets –STO-3G, 3-21G, 3-21+G and 6-31G* - *ab initio* methods (preliminary ideas).

UNIT IV - APPLIED ELECTROCHEMISTRY II

Objective: To study the EMF and its applications.

EMF – Electrochemical series and significances Reversible cells – representation – reaction for metal – metal ion, gas-ion, metal – sparingly soluble salt and redox electrodes. Standard cells – Weston Cadmium cell – thermodynamics of reversible / irreversible cells. Calculation of ΔH, ΔG, ΔS and equilibrium constant of cell reaction.

Nernst equation – Concentration cells- Expression for EMF of electrolyte concentration cells with and without transference. Liquid junction potential. Application of EMF measurements – determination of solubility product-determination of pH using quinhydrone, hydrogen, Glass electrodes – potentiometric titrations: acid-base,

oxidation reduction and precipitation titrations – Corrosion – Theory (electrochemical) and prevention.

UNIT V: BIOPHYSICAL CHEMISTRY

Objective: *To have an idea about biophysical chemistry*

Thermodynamics in biology – energy flux – transfer of potentials and coupled reactions role of singlet oxygen in biology – general principles of function and structural organization in bioenergetic fundamental reactions – structure of membranes (introductory aspects only) – solute transport across membranes – membrane potentials – ion pumps – biophysical applications of Moussbauer effect.

REFERENCES:

1. Quantum Chemistry, Donald A. Mcquire, Viva Books. 2011
2. Quantum Chemistry, A.B. Samigrahi, Books and Allied PVT Ltd, 2010.
3. Introductory Quantum Chemistry, A.K. Chandra, 4th Edn., 2001, Tata McGraw Hill.
4. Quantum Chemistry – IRA N. Levin, 6th Edn., PHI Learning PVT Ltd., New Delhi. 2009.
5. Molecular Quantum Mechanics, Atkins P W and R S Friedman, 3rd Edn.,Oxford University Press, 1996.
6. Modern Quantum Chemistry. Introduction to Advanced Electronic Structure Theory, Szabo A and N S Ostuld, Tata McGraw Hill, New York, 1982.
7. Principles of Physical Chemistry, Puri, Sharma and Pathania, Vishal Publications, 2008.

IV SEMESTER			
DSC11	ADVANCED TOPICS IN CHEMISTRY		18PCCH42
Hrs / Week: 5	Hrs / Sem.: 75	Hrs / Unit: 15	Credit: 4

UNIT I: GREEN CHEMISTRY

Green chemistry-relevance and goals, Anastas' twelve principles of green chemistry – Tools of green chemistry: alternative starting materials, reagents, catalysts, solvents and processes with suitable examples. prevention/minimization of hazardous/toxic products; designing safer chemical – different basic approaches to do so; selection of appropriate auxiliary substances (solvents, separation agents), green solvents, solventless processes, immobilized solvents and ionic liquids; energy requirements for reactions – use of microwaves, ultrasonic energy; selection of starting materials – designing of biodegradable products; prevention of chemical accidents; strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

UNIT II: NANO CHEMISTRY

Background to Nanoscience – Scientific revolution – Atomic Structure and atomic size, emergence and challengs of nanoscience – Introduction to Nanostructures: Carbon Nanotubes (CNT), Graphenes, Fullerenes, Quantum Dots and Semiconductor Nanoparticles – Introduction to metal based nanostructures (nanoparticles, nanowires, nanorod) – Introduction to Polymer based Nanostructures –Coreshell, dendrimers –Applications of nanomaterials (chemical synthesis, nanomedicine).

Nanoscience and Interface: Intermolecular Forces, Van der Waals forces (Kessorn, Debye, and London Interactions). Dynamic properties of interfaces. Contact angle. Brownian motion and Brownian Flocculation, Surface free energy.

UNIT III: SUPRAMOLECULAR CHEMISTRY

Supramolecular chemistry: Concepts, Cation binding, Binding of anions, Neutral molecules, Methods, Self-Assembly, Artificial enzymes, Molecular devices, Molecular machines.

UNIT IV: BIOPHYSICAL CHEMISTRY

Thermodynamics in biology – energy flux – transfer of potentials and coupled reactions role of singlet oxygen in biology – general principles of function and structural organization in bioenergetic fundamental reactions – structure of membranes (introductory aspects only) – solute transport across membranes – membrane potentials – ion pumps – biophysical applications of Moussbauer effect.

UNIT IV: DRUG DESIGN

Transcriptomics – probes – Northern hybridization – differential display – microarrays – types of microarray – designing a

micro array – cDNA microarray experimental – micro array data variability – Normalization – image analysis.

Metabolomics – reconstruction of metabolic pathway from complete genome sequence – metabolic pathway databases.

Pharmacogenomics – Drugs – agonist – antagonist – inhibitor – drug receptor – types – Drug designing – structure based drug design – drug discovery and development process – pharmacokinetics – simple nucleotide polymorphism – benefits and limitations.

Cheminformatics: Prediction of properties – Estimation of log $P_{o/w}$, log S & toxicity – Prediction of spectral properties – chemical shift and mass spectra – Prediction of chemical reactions.

REFERENCES:

1. Green Chemistry, V. K. Ahluwalia, 2nd edition, Ane's book Pvt Ltd.
2. Chemistry of nanomaterials: Synthesis, properties and applications by CNR Rao et.al. 2.
3. Nanoparticles: From theory to applications – G. Schmidt, Wiley Weinheim 2004.
4. A.W. Adamson and A.P.Gast, Physical Chemistry of surfaces, Wiley Interscience, NY 2004.
5. P.C Hiemen and R.Rajgopalan, Principle of colloid and surface Chemistry, NY Marcel Dekker, 1997.
6. M. J. Rosen, Surfactant and Interfacial phenomena, Wiley Inter Science Publication, NY 2004.
7. Handbook of Molecular Descriptors, R. Mannhold, H. Kubinyi, H. Timmerman (Eds) VCH Verlag 2002
8. Principles of Physical Chemistry, Puri, Sharma and Pathania, Vishal Publications, 2008.
9. Molecular Modeling, Principles and Applications, Andrew R. Leach, II Edition, 2001, Dorset Press, Dorchester, Dorset.
10. Cheminformatics, Johann Gasteiger and Thomas Engel, 2003, Wiley VCH, Weineim.
11. Introduction to Chemiformatics, Andrew.R. Leach and Valeric J Gillet, 2007, Springer.

IV SEMESTER			
C12-P	**PROJECT**		**15PCHP41**
Hrs / Week : 8	**Hrs / Sem : 75**	**Hrs / Unit : 15**	Credit : 6 **Credit : 8**

Objective:

Every PG student is required to prepare the project subject related – based on the guidelines of his / her project guide.

The following are the guidelines to be adhered to

- The project should be an individual one
- The language for the project is **English**
- The Minimum number of pages should be **60**
- Project observations, suggestions and conclusion shall form part of the project.
- The Projects will be evaluated both by the Internal as well as External Examiner each for 100 marks. The distribution of mark should be **60 marks for the Project Report and 40 marks for the Viva-voce Examination**. The Division of marks for the Project Report is as mentioned below:

Particulars	**Internal Examiner**	**External Examiner**
Wording of Title	5	5
Objectives/ Formulation including Hypothesis	5	5
Review of Literature	10	10
Relevance of Project to Social Needs	5	5
Methodology/ Technique/ Procedure Adopted	20	20
Summary/ Findings/ Conclusion	5	5
Bibliography/ Annexure/ Foot notes	10	10
Total	**60**	**60**

The average mark of Internal and External Examiner is considered as marks of project report.

IV SEMESTER			
CE4A	**MEDICINAL CHEMISTRY**		**15PCHE4A**
Hrs / Week: 3	**Hrs / Sem.: 45**	**Hrs / Unit: 9**	**Credit: 3**

UNIT I: Introduction

Objective: *To get an introductory idea about pharmacology and drugs*

Drugs -definition, Requirements of an ideal drug -Sources – Historical evolution of drugs – Nomenclature of drugs – Heterocyclic – Non-stereo chemical – Chirality of drugs - Terminology & description of the terms –Pharmacology, Pharmacokinetics, Pharmacodynamics, Metabolites, Antimetabolites and Pharmacophore - Chemical structure –therapeutic actions.

UNIT II: CARDIOVASCULAR DRUGS

Objective: *To study about different cardiovascular and vasopressor drugs and their activity*

Cardiovascular drugs – classification –structure and mechanism of action of digitoxin.

Vasopressor drugs – structure, synthesis and mode of action of prenylamine.

UNIT III - ANTIBIOTICS

Objectives*: To study about the structure and synthesis of antibiotics.*

Classification - β-Lactam Antibiotics – Penicillin (Structural Elucidation). Aminoglycoside Antibiotics – Streptomycin, Neomycin, Kanamycin (Structure, Mode of action and SAR) – Synthesis and Structural Elucidation of Chloramphenicol - Tetracyclines -Salient Features, Nomenclature and General Characteristics - Newer Tetracyclines.

UNIT IV: ANTIMYCOBACTERIAL DRUGS

Objective: *To study about different antimycobacterial drugs and their activity*

Antimycobacterial drugs – Classification – First line drugs- pyrazinamide – Second line drugs – Synthesis and mechanism of action of oflaxacin, ciprofloxacin.

UNIT-V: STRUCTURE ACTIVITY RELATIONSHIP (SAR)

Objective: To have a basic idea about Drug Designing and SAR

Economic aspects of drug designing – Procedures followed in drug designing – Lead based methods – Approaches to lead discovery – Drug discovery without a lead-*de novo* drug designing – Structure Activity Relationships: Quantitative analysis of structure activity relationships – Hansch Paradigm for pharmaceuticals

REFERENCES:

1. Organic Chemistry, I.L. Finar, Vol II, ELBS, 1975.
2. Burger's Medicinal Chemistry and Drug Discovery Vol. – I, 5thEdn. John Wiley & Sons, New York.
3. The Prostaglandins, P.M. Ramwell, Vol. I Plenum press , 1973.
4. Organic Chemistry of Natural Products, Gurdeep Chatwal, Vol. –II, Himalaya Pub. House, Bombay 1985.
5. Chemistry of organic drugs, V.Vaidhyalingam . I Edn. (Thailambigai Publications), 2000.
6. An introduction to Medicinal Chemistry, Graham L.Patrick, Oxford University press, New York, 1995.
7. Instant notes: Medicinal Chemistry, G. Patrick, Series Ed, B. D. Hames. I Indian Edn, Viva Books Pvt. Ltd. New Delhi, 2002.
8. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press, 1992
9. Drug Designs - A Series of Monographs in Medicinal Chemistry, Edited by A. J. Ariens. Ist Edition, Vol. I, II, V, VIII & IX (only relevant chapters). Academic Press, An Imprint of Elsevier, 2009
10. Medicinal Chemistry, AshutoshKar, New Age International Publishers, 2007
11. The Organic Chemistry of Drug Design and Drug action R. Silverman, (Ed) Academic Press, 2004

UNIT I: CHEMISTRY OF DRUGS

Drugs – definition, Requirements of an ideal drug – Sources – Historical evolution of drugs – Nomenclature of drugs – Heterocyclic – Non stereo chemical – Chirality of drugs – Terminology & description of the terms –Pharmacology, Pharmacokinetics, Pharmacodynamics, Metabolites, Antimetabolites and Pharmacophore – Chemical structure –therapeutic actions.

UNIT II: SEDATIVES AND HYPNOTICS

Introduction, classification, Barbiturates, Non barbiturates, Mode of action of Barbiturates, Mechanism of action, Barbiturates vs Benzodiazepines, structure-activity relationship, Barbiturates vs dissociation constant, substitution on hetero atoms in Barbiturates, OH– catalyzed degradation of Barbiturates, specific mechanism of action of some sedatives and hypnotics.

UNIT III: AUTONOMIC DRUGS

Classification, Sympathomimetic drugs, mechanism of action, Structure activity relationship, Beta Adrenergic Receptor Stimulants, mechanism of action, Adrenergic Receptor Blocking agent, Alpha Adrenergic Blocking agent, mechanism of action, Beta Adrenergic Blocking agent, First generation beta blockers, second generation beta blockers, third generation beta blockers, Alpha and Beta Adrenergic Receptor Blocking agent.

UNIT IV: DIURETICS

Introduction, classification, Mercurial Diuretics, Non Mercurial Diuretics, Thiazides, Carbonic Anhydrase inhibitors, Loop and High-ceiling Diuretics, Aldosterone inhibitors, Pyrimidine Diuretics, Osmotic Diuretics, Acidotic Diuretics, Miscellaneous Diuretics.

UNIT V: ANTIHISTAMINES AND ANTIPARKINSONISM AGENTS

Antihistamines: Introduction, classification, Histamine H_1-Receptor Antagonists, Aminoalkyl ethers, Ethylene diamines, Phenothiazine derivatives, Prevention of Histamine release, mechanism of action, Histamine H_2 Receptor Blockers, mechanism of action.

Antiparkinsonism agents: Introduction, Etiology, Parkinsonism produced by MPTP, classification, Piperidine analogues, mechanism of action, Pyrrolidine analogues, mechanism of action, miscellaneous drugs, mechanism of action.

REFERENCES:

1. Organic Chemistry, I.L. Finar, Vol II, ELBS, 1975.
2. Burger's Medicinal Chemistry and Drug Discovery Vol. – I, 5thEdn. John Wiley & Sons, New York.
3. The Prostaglandins, P.M. Ramwell, Vol. I Plenum press , 1973.
4. Organic Chemistry of Natural Products, Gurdeep Chatwal, Vol. – II, Himalaya Pub. House, Bombay 1985.
5. Chemistry of organic drugs, V.Vaidhyalingam . I Edn. (Thailambigai Publications), 2000.
6. An introduction to Medicinal Chemistry, Graham L.Patrick, Oxford University press, New York, 1995.
7. Instant notes: Medicinal Chemistry, G. Patrick, Series Ed, B. D, Hames. I Indian Edn, Viva Books Pvt. Ltd. New Delhi, 2002.
8. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press, 1992.
9. Drug Designs – A Series of Monographs in Medicinal Chemistry, Edited by A. J. Ariens. Ist Edition, Vol. I, II, V, VIII & IX (only relevant chapters). Academic Press, An Imprint of Elsevier, 2009.
10. Medicinal Chemistry, AshutoshKar, New Age International Publishers, 2007.
11. The Organic Chemistry of Drug Design and Drug action R. Silverman, (Ed) Academic Press, 2004.

IV SEMESTER			
CE4B	**RATIONAL DRUG DESIGN**		**15PCHE4B**
Hrs / Week: 3	**Hrs / Sem.: 45**	**Hrs / Unit: 9**	**Credit: 3**

UNIT – I: INTRODUCTION

Objective*: To study about the thermodynamic calculations of molecular descriptors*

Electronic, Steric and Hydrophobic substituents constant – Structural and theoretical parameters – Bioisostreism – Wilson

method and its significance – Acid base properties, ionization – partition coefficients (hydrophobicity) – Hammett constants – Taft's steric factor – resonance effect – inductive effect – Masca Model of pharmacochemistry.

Routes of drug administration – External (Oral, Sublingual) – Parenteral – Intravenous and Intrarterial, Intramuscular, Subcutaneous, Intraperitoneal, Nasal, Tropical, Inhalation, Intrathecal, Ophthalmic.

UNIT – II: **DRUGS ACTION**

Objective*: To study about the drug action*

Basic concepts – Mechanism of drug action – Common promoities – Reversal of prodrugs – chemical and enzymatic – Application of prodrug approach to alter taste and odour reduction of pain at injection site – reduction of gastrointestinal irritability – Alteration of drug solubility – increasing chemical stability – Prevention of presystematic metabolism – Prolongation of drug action – site specific drug delivery – Reduction in drug toxicity – Alteration of drug metabolism – soft drugs – design of soft drugs.

UNIT – III: QSAR

Objective*: To have an idea about QSAR and Its applications*

QSAR – Hansch& Free – Wilson Analysis – Validation and selection of QSAR models – Nonlinear QSAR models – Dissociation and ionization – application of QSAR analysis – Scope & limitation – Similarity of QSAR, HQSAR, Binary QSAR & other approaches.

3D – QSAR – Model evaluation – Distribution of activities in Physicochemical property space – Assumption in 3D – QSAR – Bioactive conformation and biological activity – COMFA, COMSIA & ALMOND.

UNIT – IV: MOLECULAR DESCRIPTORS, DOCKING AND SCORING

Objective: *To know about molecular descriptors, docking and scoring*

Molecular descriptors – types – 2D and 3D descriptors – topological indices – field based descriptors

Docking techniques – protein structure – rigid docking – docking with flexible ligands – flexible protein docking.

Scoring techniques – force field scoring – regression based scoring – knowledge base scoring – complementary score – comparison of scoring function – consensus scoring – applications – docking as a modeling tool: understanding the selectivity of thrombin/matriptase inhibitors – docking as an *insilico* screening tool – discovery of Bcl – 2 inhibitors.

UNIT – V PHARMACOKINETICS AND DRUG METABOLISM

Objective*: To understand the basic concepts of pharmacokinetics and transport of drug across biological membrane*

Pharmacokinetics and its role in drug discovery – drug absorption Distribution – Metabolism – Excretion ADME.

Drug metabolism – Oxidation (saturated carbon atoms, olefinic bonds, aromatic rings, carbon – nitrogen centres, carbon oxygen and

carbon – sulphurcentres) – Reduction (Carbonyl, Nitro, Azo groups, N – oxides, Disulfides and sulfoxides) – hydrolysis – Conjugation (Glucuronide, sulfate, Glycine, Glutamine, Methylation, acetylation and Glutathione conjugation)

REFERENCES:

1. Introduction to Molecular Modeling from Theory to Application, DimitriosVlachakis, 2007
2. Pharmacokinetic Optimization in Drug Research, B. Testa, H. van de Waterbeemd, G. Folkers, R Guy (Eds) VCH Verlag, 2002
3. Pharmacokinetics and metabolism in Drug Design, D.A. Smith, H. van de Waterbeemd, D.K. Walker John Wiley & Sons, 2000
4. Pharmacogenomics The Search for Individual Therapies, J. Licinio, M.L. Wong VCH Verlag, 2002
5. Drug Bioavailability: Estimation of Solubility, Permeability, Absorption, and Bioavailability, H van de Waterbeemd, H. Lennernäs, P. Artursson, P. Manhold, H. Kubinyi, G. Folkers, VCH Verlag 2003
6. The Organic Chemistry of Drug Design and Drug action, Silverman, (Ed) Academic Press 2004.
7. Design of Drugs: Basic Principles and Applications, J.H. Poupaert Marcel Dekker, 2002
8. Structure based Drug Design, P. Veerapandian (Ed) Marcel Dekker, 1997.
9. Modern Methods of Drug Discovery, A. Hillisch, R. Hilgenfeld (Eds) Springer Verlag, 2003
10. Text Book of Drug Design and Discovery, P. Krogsgaard – Larsen, T. Liljefors, U. Madsen (Eds) Taylor & Francis 2002
11. Drug Discovery and Evaluation, H. Vogel (Ed) Springer Verlag, 2002
12. 3D QSAR in Drug Design: Ligand – Protein Interactions and molecular similarity by H. Kubinyi, Y.C. Martin, G.Folkers (Eds) Kluwer Academic Publishers, 1998
13. Quantitative Structure – Activity Relationship (QSAR): Models and Mutagens and Carcinogens, R. Benigni (Ed) CRC Press, 2003
14. Handbook of Molecular Descriptors, R. Mannhold, H. Kubinyi, H. Timmerman (Eds) VCH Verlag 2002

III & IV SEMESTER			
CP4	INORGANIC CHEMISTRY PRACTICAL II		15PCHC4P1
Hrs / Week: 3	Hrs / Sem.: 60	Hrs / Year: 120	Credit: 2

I Gravimetric estimation and qualitative analysis

1. Estimation of copper (V) and nickel (G)
2. Estimation of copper (V) and zinc (G)
3. Estimation of Iron (V) and Nickel (G)
4. Estimation of barium (V) and calcium (G)

II Preparation of Inorganic Complexes

i. Tris -acetylacetonato iron(III)

ii. $Ni(dmg)_2$

iii. Potassium ferrioxalate

iv. Cis- Chromiumdioxalatodihydrate

v. Tri(acetylacetonato)manganese(III) $Mn(acac)_2$

vi. Prussian blue

vii. Tetrammminecopper(II) sulphate

viii. hexaamine cobalt(III) chloride

REFERENCES:

1) Vogel's Qualitative Inorganic Analysis, 7th edition, Pearson, 2006.
2) College Practical Chemistry, V K Alhuvalia, Sunita Dingra, 1-Edition, University Press, 2005
3) A collection of interesting general chemistry experiments, A. J. Elias, University Press, 2002
4) Inorganic Chemistry Practical, Deepak Pant, e-book, Book-Rix edition.

III & IV SEMESTER			
CP5	ORGANIC CHEMISTRY PRACTICAL – II		15PCHC4P2
Hrs / Week: 3	Hrs / Sem.: 60	Hrs / Year: 120	Credit: 2

I Preparation of drugs and characterization.
(Students are expected to verify the drugs by either physical constants or UV visible spectral method)

1. Phenacetin
2. Paracetamol
3. Dichloramine T
4. Fluorescein
5. Benzimidazole
6. Benzotriazole

II Extraction and analysis of the following natural products

1. Euginol from clove.
2. Piperine from black pepper
3. Caffeine from tea leaves
4. Lycopenes from tomato
5. Carotene from carrot

III. Chromatographic techniques
Separation of mixtures

1. Aniline and m-nitro toluene
2. Benzophenone and benzoic acid and checking their R_f values by
3. Identification of amino acid with the help of TLC or PC. Calculation of R_f value of individual amino acid
4. Identification of sugar (glucose, fructose, sucrose) with the help of TLC or PC. Calculation of R_f value.

REFERENCES:

1. Lab Experiments in Organic Chemistry, Arunsethi, New Age International Publishers, 2010.
2. The Systematic Identification of Organic Compounds R.L. Shriner, C.K.F. Hermann, T.C. Morrill, D.Y. Curtin & R.C. Fuson John Wiley & Sons, Inc., 1997.
3. Identification of organic compounds. By N. D. Cheronis and J. B. Entrikin. Interscience Publishers, New York, 1963.
4. Organic Cum Practical Hand Book Of Organic Chemistry, B J Hassard
5. Organic Experiments, Louis F. Fisser, Kenneth Williamson, D.C. Heath and company, 1992.
6. A Hand Book Of Organic Analysis: Qualitative and Quantitative, Hans Thacher Clarke,1916.
7. Experimental Organic Chemistry, H Dubont Durst And George W Gokal, 2nd Edn., New York: McGraw-Hill, 1987.
8. Practical Organic Chemistry, F G Mann and B C Saunders, 4th Edn., Pearson Education Ltd., 2009.
9. Textbook Of Practical Organic Chemistry, A I Vogel, Prentice Hall; 5th Edn., 1989.
10. Systematic Organic Chemistry, Modern Methods of Preparation and Estimation. By W.M. Cumming, I. Vance Hopper, and T. Sherlock Wheeler, London, 1923.

III & IV SEMESTER			
CP6	PHYSICAL CHEMISTRY PRACTICAL II		15PCHC4P3
Hrs / Week: 3	Hrs / Sem.: 60	Hrs / Year: 120	Credit: 2

1. Verification of Ostwald's dilution law
2. Primary salt effect (Course Work)
3. Kinetics of persulphate – iodide reaction in solution
4. Study of distribution of benzoic acid
5. Comparison of acid strength by ester hydrolysis
6. Determination of heat of solution of naphthalene – toluene system
7. Determination of heat of solution of oxalic acid – water system
8. Determination of heat of solution of ammonium oxalate – water system
9. Adsorption of acetic acid / oxalic acid on activated charcoal – verification of Freundlich isotherm determination of unknown concentration
10. Determination of partial molar volume of solute (eg. KCl) and solvent in a binary mixture.
11. Determination of stoichiometry and stability constant of inorganic and organic complexes.
12. **Computational Chemistry (course work)**

Draw the structure of simple molecules (CH_4 / Ethane / Water/ toluene/ benzene/ HCHO) in:

- Gauss View
- Chem3D

Observe the amount of effort required in each case.

Use GaussView version of the above molecules as .mol file and read it with Gaussian.
Run geometry optimizations using
a.Hartree-Fock (HF / STO-3G)
b. HF / 3-21G
c.HF / 6-31G*
Observe the time taken for running each molecule. Save the output file.

Read the .mol file with Gauss View and set up a Gaussian job for the above molecules and run geometry optimization using DFT with B3LYP / 6-31G* (reasonable accuracy) basis set. Save the output file.

REFERENCES:

www.gaussian.com

IV SEMESTER		
P-VII	INORGANIC CHEMISTRY PRACTICAL II	18PCCH4P1
Hrs / Week: 4	Hrs / Sem.: 60	Credit: 2

I Gravimetric estimation and qualitative analysis

1. Estimation of copper (V) and nickel (G)
2. Estimation of copper (V) and zinc (G)
3. Estimation of Iron (V) and Nickel (G)
4. Estimation of barium (V) and calcium (G)

II Preparation of Inorganic Complexes

i. Tris- acetylacetonato iron(III)

ii. $Ni(dmg)_2$

iii. Potassium ferrioxalate

iv. Cis- Chromiumdioxalatodihydrate

v. Tri(acetylacetonato)manganese(III) $Mn(acac)_2$

vi. Prussian blue

vii. Tetrammminecopper(II) sulphate

viii. hexaamine cobalt(III) chloride

REFERENCES:

1) Vogel's Qualitative Inorganic Analysis, 7th edition, Pearson, 2006.
2) College Practical Chemistry, V K Alhuvalia, Sunita Dingra, 1 Edition, University Press, 2005
3) A collection of interesting general chemistry experiments, A. J. Elias, University Press, 2002
4) Inorganic Chemistry Practical, Deepak Pant, e book, Book Rix edition.

IV SEMESTER		
P-VIII	GREEN CHEMISTRY PRACTICAL	18PCCH4P2
Hrs / Week: 4	Hrs / Sem.: 60	Credit: 2

I. Preparation of compounds using green chemistry

1. Preparation of benzopinacolone
2. Preparation of 1, 1-bis-2-naphthol
3. Synthesis of adipic acid
4. Synthesis of biodiesel
5. Preparation of Manganese(III) acetylacetonate, $Mn(acac)_3$ or $Mn(C_5H_7O_2)_3$
6. Preparation of Iron(III) acetylacetonate, $Fe(acac)_3$ or $Fe(C_5H_7O_2)_3$

II. Spot test using green Chemistry-Basic radicals (Pb^{2+}, Cu^{2+}, Cd^{2+}, Bi^{3+}, Co^{2+}, Ni^{2+}, Mn^{2+}, Zn^{2+}, Ba^{2+}, Ca^{2+}, Sr^{2+}), Acid radicals (F^-, Br^-, I^-, NO_2^-, NO_3^-, S^{2-}, SO_3^{2-} SO_4^{2-}, SCN^-)

III. Identification of N,S, Cl, Br and I using Green Chemistry

REFERENCES:

1. Lab Experiments in Organic Chemistry, Arunsethi, New Age International Publishers, 2010.
2. The Systematic Identification of Organic Compounds R.L. Shriner, C.K.F. Hermann, T.C. Morrill, D.Y. Curtin & R.C. Fuson John Wiley & Sons, Inc., 1997.
3. Identification of organic compounds. By N. D. Cheronis and J. B. Entrikin. Interscience Publishers, New York, 1963.
4. Organic Cum Practical Hand Book Of Organic Chemistry, B J Hassard
5. Organic Experiments, Louis F. Fisser, Kenneth Williamson, D.C. Heath and company, 1992.
6. A Hand Book Of Organic Analysis: Qualitative and Quantitative, Hans Thacher Clarke,1916.
7. Experimental Organic Chemistry, H Dubont Durst And George W Gokal, 2nd Edn., New York: McGraw-Hill, 1987.
8. Practical Organic Chemistry, F G Mann and B C Saunders, 4th Edn., Pearson Education Ltd., 2009.
9. Textbook Of Practical Organic Chemistry, A I Vogel, Prentice Hall; 5th Edn., 1989.
10. Systematic Organic Chemistry, Modern Methods of Preparation and Estimation. By W.M. Cumming, I. Vance Hopper, and T. Sherlock Wheeler, London, 1923.
11. Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST.

IDC SUBJECTS OFFERED BY DEPARTMENT OF CHEMISTRY TO OTHER MAJOR STUDENTS II SEMESTER			
IDC-1	INDUSTRIAL CHEMISTRY		18PICH21
Hrs / Week: 3	Hrs / Sem.:45	Hrs / Unit:9	Credit:3

UNIT I: METALLURGY

Minerals – Ores – Extraction – Concentration – Froth floatation process – Zone refining – Magnetic separation. Extraction – Aluminium from bauxite, Nickel by Mond's process, Lead from galena, – Uses.

Alloys – Composition and uses – Nickel iron alloys Nickel chromium alloys.

Corrosion – Types – Chemical corrosion – Factors affecting chemical corrosion – Methods of preventing corrosion – Electroplating, Hot dipping.

UNIT II: CEMENT INDUSTRY

Composition – Classification – Natural and Artificial cement. Manufacture – Wet process, Dry process.

Portland cement – Manufacture – Advantages, Disadvantages – ISI specification of Portland cement. Gypsum – Role of gypsum in cement.

High alumina cement – White Portland cement – Blended cement – Uses.

Cement industries in India.

UNIT III: PYROTECHNIQUES

Match industry: Safety matches – Composition of the match head, fireworks – colored matches.

Explosives: Classifications – primary explosives – Preparation – lead azide, DDNP, Tetryl and EDNA. High explosives – Preparation of TNT, picric acid, Ammonium picrate, GTN, PETN, RDX.

Propellants – Manufacture of liquid and solid propellants.

UNIT IV: MANUFACTURE OF DAY TO DAY ARTICLES

Manufacture of Naphthalene balls – Wax candles – Shoe polish – Plaster of Paris.

Preparation and uses of Hair dye – Shampoo – Sun tan lotion – Face powder.

Essential oils in cosmetics – Properties and uses – Eugenol – Geraniol – Sandalwood oil – Eucalyptus.

Printing Inks – Raw materials, Manufacture, Properties, Uses, Types– Lithographic – Flexographic – Screen inks.

UNIT V: PETROCHEMICALS

Refining of petroleum – Composition and uses of main petroleum fractions – Cracking – Thermal Cracking, Catalytic cracking – Advantages – Octane number – Antiknock agents – Unleaded petrol – Cetane number – Anti diesel knock agents – Flash point – Synthetic petrol. Petrochemicals – Manufacture and industrial uses of Methanol

– Ethanol – Acetone. Manufacture – Ethanol from sugarcane. Composition - Rectified spirit – Absolute alcohol.

REFERENCES:

1. Industrial Chemistry – B.K.Sharma, 2003, Goel Publishing House, Meerut.
2. Industrial Chemicals – Faith etal, Wiley Interscience, New York.
3. Chemical Process Industries – R.N. Shreve, 2000; Tata McGraw Hill Publishing Company, Mumbai.
4. James A. K., Reigel's Handbook of Industrial Chemistry 9th Edition, CBS Publication 1997.
5. Principles of Industrial Chemistry, C. A. Clausen and G. Matts.
6. Chakrabarty B.N. (1981): Industrial chemistry, Oxford & IBH publishing Co., New Delhi.

III SEMESTER			
IDC-2	INTRODUCTION TO CHEMINFORMATICS		18PICH31
Hrs / Week: 3	Hrs / Sem.: 45	Hrs / Unit: 9	Credit: 3

UNIT I: Computer Representation of Molecular Structure and Retrieval

Scope of Cheminformatics – Hierarchy of representation of a molecule – Virtual molecules – Molecular graphs – Graph and subgraph – Line notations – SMILES construction – Matrix representation – Adjacency matrix – Distance matrix – Connection table – File formats – Mol files – PDB files – Canonical representation. Substructure – Sub graph isomerism – Structural keys – Fingerprints – Matching of molecular structures.

UNIT II: Databases and data sources in Chemistry

Classification of databases – Chemical Abstracts System (CAS) – SCISEARCH & MEDLINE – Factual databases – property databases – Beilstein and Gmelin – Crystal structure databases – CSD, ICSD – Structure databases – NCI – Classification of Scientific Literature – primary, secondary and tertiary literature – Online databases – Pubmed – ZINC database.

UNIT – III: Chemical Information Searches

Full structure search – Substructure search – Screening methods – Algorithms for Subgraph Isomorphism – Practical aspects of structure searching. Similarity search process – Object selection – Descriptor selection and Encoding – Query object specification – Similarity scores.

UNIT –IV: Molecular Descriptors

2D Descriptors - Physicochemical properties – Topological description – Kappa shape indices – Electrotopological state indices – Atom pairs and Topological Torsions – Extended connectivity Fingerprints – 3 D descriptors – 3D structure generation – 3D Autocorrelation - Chirality descriptors – Quantitative Descriptions of chirality – BCUT descriptors – HYBOT descriptors.

UNIT V: Application of Cheminformatics

Prediction of properties – Estimation of log Pow, log S & Toxicity – Prediction of chemical reactions – Computer assisted synthesis design – Drug design – Target identification & validation – Lead finding

and optimization – Design of combinatorial libraries – Structure based and ligand based drug design.

REFERENCES:

1. Cheminformatics: concepts, methods, and tools for drug discovery (methods in molecular biology) Bajorath, J., Ed.; Humana Press: Totowa, NJ, 2004.
2. Bioinformatics: Sequence and Genome Analysis, Mount, D), Cold Spring Harbor Laboratory Press, New York, 2004
3. Gasteiger, J.; Engel, T. Cheminformatics: a textbook. Wiley-VCH, Weinheim, Germany, 2003.
4. Molecular Modeling, Principles & Applications, Andrew R. Leach
5. Bioinformatics – a practical guide to the analysis of Genes and Proteins, Baxevanis, A.D. and Francis Ouellellette, , John Wiley & Sons, UK, 1998
6. Molecular Modeling, Principles and Applications, II Edition, Andrew R. Leach, Dorset Press, Dorchester, Dorset, 2001.
7. Lednicer, D. (1998). Strategies for Organic Drug Discovery Synthesis and Design. Wiley International Publishers

SCHEME OF EXAMINATIONS UNDER CBCS

The medium of instruction in all PG courses is English and students shall write the CIA Tests and Semester Examinations in English. However, if the examinations were written in Tamil, the answer papers will be valued.

DISTRIBUTION OF MARKS FOR CIA AND SEMESTER EXAMINATIONS FOR POSTGRADUATE COURSES

SUBJECT	TOTAL MARKS	CIA TEST	SEMESTER EXAMINATION	PASSING MINIMUM		
				CIA EXAM.	SEM. EXAM.	OVER ALL
Theory	100	25	75	Nil	38	50
Practical	100	40	60	Nil	30	50
Project	100	Nil	Report - 60 marks Viva Voce - 40 marks	Nil	50	50

DIVISION OF MARKS FOR CIA TEST

SUBJECT	MARKS	ASSIGNMENT OR SEMINAR FOR PG	REGULARITY	RECORD NOTE	TOTAL MARKS
Theory	20	5	--	--	**25**
Practical	30	--	5	5	**40**

1. The duration of each CIA Test is ONE hour and the Semester Examination is THREE hours.
2. Three CIA tests of 20 marks each will be conducted and the average marks of the best two tests out of the three tests will be taken.
3. The I test will be based on the first 1.5 units of the syllabus, the II test will be based on the next 1.5 units of the syllabus and the III test will be based on the next 1.5 units of the syllabus.
4. Two assignments for Undergraduate, Certificate, Diploma and Advanced Diploma Courses and two assignments OR two seminars for Postgraduate Courses.
5. The duration and the pattern of question paper for practical examination may be decided by the respective Boards of Studies. However, out of 60 marks in the semester practical examination, 10 marks may be allotted for record and 50 marks for practical.
6. Three internal practical tests of 25 marks each will be conducted for science students in the even semester and the best two out of the three will be taken. The total 50 marks of the best two tests will be converted to 30 by using the following formula:

$$\left(\begin{array}{c}\text{Marks secured in the first best Practical Test (Out of 25)} \\ + \\ \text{Marks secured in the next best Practical Test (out of 25)}\end{array}\right) \text{X } 0.6$$

7. The Heads of Science Departments are requested to keep a record of attendance of practicals for students to assign marks for regularity.

QUESTION PAPER PATTERN FOR CIA TEST (THEORY)

Duration: 1 Hr **Maximum Marks: 20**

Section	Question Type	No. of Questions & Marks	Marks
A	No Choice Answer should not exceed 75 words	2 Questions 2 marks each	2 x 2 = 4
B	Internal choice (Either or type) Answer should not exceed 200 words	2 Questions 4 marks each	2 x 4 = 8
C	Open Choice (Answer ANY ONE out of Two) Answer should not exceed 400 words	1 Question 8 marks	1 x 8 = 8
		TOTAL	**20 MARKS**

QUESTION PAPER PATTERN FOR SEMESTER EXAMINATION (THEORY)

Duration: 3 Hrs **Maximum Marks: 75**

Section	Question Type	No. of Questions & Marks	Marks
A	No Choice Answer should not exceed 75 words	10 Questions - 2 marks each (2 Questions from each unit)	10 x 2 = 20
B	Internal choice (Either or type) Answer should not exceed 200 words	5 Questions with internal choice. Each carries 5 marks (Two questions from each unit)	5 x 5 = 25
C	Open Choice (Answer ANY THREE out of FIVE) Answer should not exceed 400 words	3 Questions out of 5 - 10 marks each (1 Question from each unit)	3 x 10 = 30
		TOTAL	**75 MARKS**