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	Department of Chemistry (PG)									
	(2017 Onwards) M.Sc. Chemistry Course structure (CBCS)									
	Course	H/W			Course	H/W	С			
	Core 1 (C1)	5	5		Core 4 (C4)	5	5			
	Core 2 (C2)	5	5		Core 5 (C5)	5	5			
	Core 3 (C3)	5	5		Core 6 (C6)	5	5			
er	Core Elective – 1			er	Core Elective – 2					
ŝ	(A/B)	3	3	est	(A/B) (CE2A/CE2B)	3	3			
Ĕ	(CE1A/CE1B)			Semester						
I Semester	Core Practical – I* (CP1)	4	-	II Se	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			
	Total	30	18		Total	30	27			
							_			
	Course	H/W			Course	H/W	С			
	Core 7 (C7)	5	5		Course Core 10 (C10)	5	5			
		5 5	5 5		Core 10 (C10) Core 11(C11)	5 5	5 5			
er	Core 7 (C7) Core 8 (C8) Core 9 (C9)	5	5	er	Core 10 (C10) Core 11(C11)	5	5			
nester	Core 7 (C7) Core 8 (C8)	5 5	5 5	nester	Core 10 (C10) Core 11(C11)	5 5	5 5			
I Semester	Core 7 (C7) Core 8 (C8) Core 9 (C9)	5 5 5	5 5 5	/ Semester	Core 10 (C10) Core 11(C11) Project (P) Core Elective – 3 (A/B)	5 5 8	5 5 6			
III Semester	Core 7 (C7) Core 8 (C8) Core 9 (C9) Non-Major Elective Core Practical – IV*	5 5 5 6	5 5 5 5	IV Semester	Core 10 (C10) Core 11(C11)	5 5 8 3	5 5 6 3			
	Core 7 (C7) Core 8 (C8) Core 9 (C9) Non-Major Elective Core Practical – IV* (CP4) Core practical – V*	5 5 5 6 3	5 5 5 -	IV Semester	Core 10 (C10) Core 11(C11) Project (P) Core Elective – 3 (A/B) (CE4A/ CE4B) Core Practical – IV* (CP4)	5 5 8 3 3	5 5 6 3 2			

\* 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)	9	9	3	300
Non-Major Elective	5	5	1	100
Total	120	90	22	2200

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

		Department of Che						
		CBCS Syllabus – M.Sc., Chem	nistry (2017		ards			
Sem	Р	Title of the Paper	Sub. Code	H/ W	С	I	Mark: E	s T
	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
		CHROMATOGRAPHY	15PCHE1A		-			
		BIOCHEMISTRY	15PCHE1B	3	3	25	75	100
Ι	CP1	INORGANIC CHEMISTRY PRACTICAL -I	15PCHC2P1	4		Exa	m – II	Sem
	CP2	ORGANIC CHEMISTRY PRACTICAL – I	15PCHC2P2	4		Exa	m – II	Sem
	CP3	PHYSICAL CHEMISTRY PRACTICAL - I	15PCHC2P3	4		Exa	m – II	Sem
	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
II	CE2B	ENZYME CHEMISTRY	15PCHE2B					
11	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
	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
III	CE3B							
	CP4	INORGANIC CHEMISTRY PRACTICAL-II	15PCHC4P1	3		Exam – IV Sem		
	CP5	ORGANIC CHEMISTRYPRACTICAL - II	15PCHC4P2	3	-	Exa	m – IV	Sem
	CP6	PHYSICAL CHEMISTRY PRACTICAL-II	15PCHC4P3	3			m – IV	Sem
	C8	ORGANIC CHEMISTRY – IV	15PCHC41	5	5	25	75	100
	C9	PHYSICAL CHEMISTRY – IV	15PCHC42	5	5	25	75	100
	Р	PROJECT	15PCHP41	8	6	0	100	100
IV		MEDICINAL CHEMISTRY RATIONAL DRUG DESIGN	15PCHE4A 15PCHE4B	3	3	25	75	100
	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	Р	Title of the memory	S Codo I	H/W	~		Mark	s
SEIM	r	Title of the paper	S. Code	п/ w	U	Ι	E	Т
Ι	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	~	Μ	AR	KS	
2 CIVI	IIILE OF THE PAPER	THE PAPER S.CODE		C	Ι	E	Т	
	DEPT. OF ENGLISH (PG)							
III	English For Business Communication	15PENN31	6	5	25	75	100	
	DEPT. OF COMPUTER	SCIENCE (P	G)					
III	Internet Concepts and Web Design	15PCSN31	6	5	25	75	100	
	DEPT. OF MATHEM	IATICS (PG)						
III	Basics in Mathematics	15PMAN31	6	5	25	75	100	
	DEPT. OF PHYS	ICS (PG)						
III	Renewable Energy Sources	15PPHN31	6	5	25	75	100	
	DEPT. OF CHEMI	STRY (PG)						
	Cheminformatics (OR)	15PCHN31A			~ =		1.0.0	
III	Applied Chemistry 15PCHN31B		6	5	25	75	100	
	DEPT. OF ZOOL	OGY (PG)						
III	Wild life management (OR)	15PZON31A	6	F	05	75	100	
111	Apiculture	15PZON31B	U	3	23	13	100	

I SEMESTER						
C1	INORGANIC CH	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<sub>2</sub>, Spinel and Rutile. Crystal defects – line and plane defects – intrinsic point defects – Schottky and Frenkel defects – Extrinsic point defects – nonstoichiometric defects. Color centres. Electronic structure of solids – Free electron and Band theory.

## UNIT II: CHEMICAL BONDING & STEREOCHEMISTRY

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

VSEPR theory – concept of hybridization & structure of molecules – Bent's rule –Apicophilicity  $d\pi$ - $p\pi$  bonds, M.O theory – symmetry and overlap – M.O diagram of HF and BeH<sub>2</sub>. Walsh diagram (triatomic molecules).

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.

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

*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<sub>5</sub>H<sub>9</sub>, nido-2,3-C<sub>2</sub>B<sub>4</sub>H<sub>8</sub>, closo-1,5-C<sub>2</sub>B<sub>3</sub>H<sub>5</sub> and closo-2,4-C<sub>2</sub>B<sub>5</sub>H<sub>7</sub>.

## UNIT IV: METAL CARBONYLS & METAL CLUSTERS.

**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)<sub>4</sub>, Fe(CO)<sub>5</sub>, Cr(CO)<sub>6</sub>, Mn<sub>2</sub>(CO)<sub>10</sub>, Co<sub>2</sub>(CO)<sub>8</sub>, Fe<sub>2</sub>(CO)<sub>9</sub> – Distinction of bridged and terminal carbonyl using IR spectra Metal nitrosyls – Structure of  $[Ir(PPh_3)_2CO(NO)Cl]^+$  and  $[Ru(PPh_3)_2(NO)_2Cl]^+$ .

#### UNIT V: NOBLE GASES, PSEUDOHALOGENS & INTERHALOGEN COMPOUNDS

**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<sub>3</sub>, ICl<sub>3</sub>, ClF<sub>3</sub>, IF<sub>5</sub>, IF<sub>7</sub>.

Polyhalide ions and polyhalides – classification – preparationproperties. 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.

#### **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
- Advanced Inorganic chemistry, F. A. Cotton, R. G. Wilkinson, 6<sup>th</sup> Edn., Wiley, 1996
- 7. Modern Inorganic Chemistry, Willam L. Jooly, Magraw-Hill, 1991.
- 8. Inorganic Chemistry, D.F.Shriver and P.W. Atkins, 4<sup>th</sup> Edn., Harper Collins, 1993.
- Modern Inorganic Chemistry, R. D. Madan & Satya Prakash, S Chand and Company, Ltd., 1<sup>st</sup> Edn., 1987.
- 10. Inorganic Chemistry, Gary L. Miessle and Donald A. Tarr, Dorling Kindersley (India) Pvt. Ltd., 3<sup>rd</sup> 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 CHE	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  $\sigma$  and  $\pi$  bonds.

Carbanion- Structure, formation, reaction and stability

Benzyne- structure, mechanism, evidence and trapping.

Carbenes: Structure, generation, reaction – addition, insertion reactions, rearrangement reactions.

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<sub>4</sub>, K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>, 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<sub>3</sub>COOH), 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), 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, KolbeSchmitt 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

# 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  $\sigma$  and  $\pi$  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.

## REFERENCES

1. Advanced Organic Chemistry, Part A: Structure and Mechanisms, F.A. Carey, R.A. Sundberg, 5<sup>th</sup>Edn., Springer, 2007.

2. Organic Reaction Mechanisms, A.C. Knipe, John Wiley& Sons Ltd. Publications, 2012.

3. Advanced Organic Chemistry, Jerry March,4<sup>th</sup> Edn., A John Wiley& Sons Ltd, 2005

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,2<sup>nd</sup> Edn.Harper & Row, 1981.

8. Stereochemistry of Organic Compounds: Principles and Applications, D. Nasipuri, 3<sup>rd</sup> Edn., New Age Pub., 2010.

9. Organic Reaction Mechanisms, V.K. Ahluwalia and Rakesh Kumar Parashar, Narosoa Publishing House, 4<sup>th</sup>Edn., 2011.

10. Palladium in Heterocyclic Chemistry, Jie Jack Li, Gordon W. Gribble, 2<sup>nd</sup> 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, 2<sup>nd</sup> Edn., McGraw-Hill Higher Education, 2002.

I SEMESTER						
C3	PHYSICAL CHEMISTRY – I 15PCHC1					
Hrs / Week: 5	Hrs / Sem.: 75	Hrs / Unit: 15	Credit: 5			

## UNIT I: THERMODYNAMICS – I

*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 –  $\Delta G_{mix}$ ,  $\Delta S_{mix}$ ,  $\Delta H_{mix}$ ,  $\Delta V_{mix}$  and  $\Delta A_{mix}$  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**

#### **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.

### **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.

## 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.

## **REFERENCES:**

- 1. Physical Chemistry, P. W. Atkins, Oxford University press, 7<sup>th</sup> Edition, 2002.
- 2. Physical Chemistry, G. M. Barrow, Tata-McGraw Hill, 5<sup>th</sup> Edition, 2003.
- 3. Physical chemistry, G. K. Vemulapalli, Prentice-Hall of India, 1997.
- 4. Thermodynamics for Chemists, S. Glasstone, D. Van Nostrand, 1965.
- 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, 4<sup>th</sup> 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 15PCHE					
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<sub>f</sub> 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; 7<sup>th</sup> Edn., 1988.

5. Thin Layer Chromatography- A laboratory Handbook, Ashworth, Stahl. E., 1<sup>st</sup> 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	BIOCHEM	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 –  $\beta$ oxidation – Synthesis of fatty acid synthase.

#### **REFERENCES**

- 1. Biochemistry, Lehinger J.CB S.Publishers, 1993.
- Biochemistry, D.Voet and J.G.Voet. 2<sup>nd</sup> 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. 4<sup>th</sup> Edn., Lippinocoth William & Willeing, 1999.
- 5. Biochemistry, U. Satyanarayana & U. Chakrapani, Books & Allied Pvt. Ltd, 1999.
- Biochemistry Lubert Stryer W. H. Freeman and company, 4<sup>th</sup> Edn., New York, 1995.
- 7. Concepts of Biochemistry, A.C. Deb,
- 8. Biochemistry, S.C. Rastogi, Ane Book (Pvt.) Ltd., 2<sup>nd</sup> Edn., 2003.
- 9. Biochemistry, Keshav Trehan, New Age International, 2<sup>nd</sup> Edn., 1990.
- 10. Biochemistry Review, U. Satyanarayana, 1<sup>st</sup> Edn., Arunabaha Sen, 2000.

II SEMESTER						
C4	INORGANIC C	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.

## 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  $\Delta$ . Application of crystal field theory in colour, spectral and magnetic properties – Jahn Teller Effect distortion.

## UNIT III: COORDINATION CHEMISTRY III

**Objective:** To study coordination chemistry

Molecular Orbital Approach-  $\sigma$  and  $\pi$  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  $\beta$  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.

### UNIT IV: COORDINATION CHEMISTRY IV

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

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 –  $\pi$  - bonding theory – Electron transfer reaction – outer sphere and inner sphere mechanism.

#### **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<sup>1</sup>, d<sup>2</sup>, d<sup>3</sup>, d<sup>4</sup>, d<sup>6</sup>, d<sup>7</sup>, d<sup>8</sup> and d<sup>9</sup> in Octahedral environment – d<sup>6</sup>, d<sup>7</sup>, and d<sup>8</sup> in tetrahedral environment, Tanabe Sugano diagram – Evaluation of  $\Delta$  and  $\beta$  values for d<sup>2</sup> (Ti<sup>2+</sup>) d<sup>7</sup> (Co<sup>2+</sup>) for octahedral systems and d<sup>3</sup> (V<sup>2+</sup>), d<sup>8</sup> (Ni<sup>2+</sup>) tetrahedral systems – Charge transfer spectra for complexes.

### **REFERENCE BOOKS:**

- 1. Principles of Inorganic Chemistry, Puri Sharma. Vishal Publishers, 2008.
- Inorganic Chemistry Principles, Structure and Reactivity, J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi,4<sup>th</sup> 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, 6<sup>th</sup> 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
- Structural methods in Inorganic Chemistry, E A V Ebsworth, David, W H Rankin, Sleptren Credock, Blackwell; 2<sup>nd</sup> 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 15PCHC2			15PCHC22
Hrs / Week: 5	Hrs / Sem.: 75	Credit: 5	

## UNIT I: STEREOCHEMISTRY

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

Chirality – prochirality – enantiotopic and diastereotopic atoms – 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.

## 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 antiaromaticity – 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.

## 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,  $\alpha$ -pyrones,  $\gamma$ -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.

#### **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  $\pi$  methane rearrangement – Photo reduction – Photochemistry of olefins – cis & trans isomerization

#### **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, 1<sup>st</sup> 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, 3<sup>rd</sup> Edn, Pearson Education Asia 2002

II SEMESTER				
C6 PHYSICAL CHEMISTRY – II 15PCHC23			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  $\rightarrow$  Product (same initial and different initial concentration) – Reversible reaction – Parallel reactions – Consecutive reaction – Chain reaction –Kinetics of H<sub>2</sub> + Br<sub>2</sub>  $\rightarrow$  2HBr Decomposition of acetaldehyde – Decomposition of ethane – Theory of reaction rate – Lindemann – Activated complex theory – Hinshelwood theory – RRK theory – Marcus theory – RRKM theory.

## 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 – 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.

## 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.

#### **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, 2<sup>nd</sup> 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, 8<sup>th</sup> 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:**

- 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).
- Instrumental Methods of Analysis Hobart H. Willard, Lynne L. Merritt Jr, John Dean, Wadsworth Publishing Co Inc; 7<sup>th</sup> Edn., 1988.
- 5. Thin Layer Chromatography- A laboratory Handbook, Ashworth, Stahl. E., 1<sup>st</sup> 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, 2<sup>nd</sup> Edition, Cambridge University Press, 2002.

II SEMESTER			
CE2B	ENZYME CHEMISTRY 15PCHE2B		
Hrs / Week: 3	Hrs / Sem.: 45	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 (lDH), 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
- Biochemistry, D.Voet and JG, Voet, John Wiley & Sons, Inc. 2<sup>nd</sup> Edn., 1995.
- 3. Fundamentals of Biochemistry, Jain J.L Chand & Co, New Delhi, 2000
- Biochemistry, Davison, V.L. & Sitlmon, D.L. 4<sup>th</sup> Ed, Lippinocoth William & Willeing, 1999
- Enzymolgy, Malcom Dixon and Edwin C. Webb Academic Press, 2<sup>nd</sup> 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

I <mark>&amp; II SEMESTE</mark> R			
CP1 INORGANIC CHEMISTRY PRACTICAL - I 15PCHC2P			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<sub>f</sub> values.

### **REFERENCES:**

- 1. Vogel's Qualitative Inorganic Analysis, 7<sup>th</sup> 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 15PCHC2P			
Hrs / Week: 4	Hrs / Sem.: 60 Hrs / Year: 120 Credi			

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, 4<sup>th</sup> Edn., F G Mann, S C Saunders, 1978.

I & II SEMESTER			
CP3 PHYSICAL CHEMISTRY PRACTICAL 15PCHC2P3			15PCHC2P3
Hrs / Week: 4	Hrs / Sem.: 60	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<sub>4</sub>Cl 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<sub>4</sub> using Debye Huckel Limiting law.

### **Potentiometric Experiments:**

9. Estimation of FAS by Potentiometric titration

10. Estimation of KMnO<sub>4</sub> 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  $\Delta G$ ,  $\Delta S$  and  $\Delta H$  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

III SEMESTER				
C7 INORGANIC CHEMISTRY - III 15PCHC3			15PCHC31	
Hrs / Week: 5	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  $\sigma$  donors – metal alkyl and aryls – Synthesis, reactions – structure and bonding in metal alkyl and aryls.

Carbon  $\pi$ - donors, chain  $\pi$ -donor ligands – olefin, acetylene and allyl  $\pi$  systems – Synthesis – structure and bonding in olefins, Zeise's salt, acetylene and  $\pi$ -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 (<sup>31</sup>P, <sup>19</sup>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. Inorganic Chemistry - Principles, Structure and Reactivity, J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi,4<sup>th</sup> 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, 1<sup>st</sup> 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, 2<sup>nd</sup> Edition, Surfside Scientific Publishers, 1992.

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

### **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  $\lambda_{max}$  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<sub>2</sub>, H<sub>2</sub>O. Vibrational frequencies – Factors affecting IR spectra – Finger print region – Fermi resonance – Applications of IR spectroscopy.

### UNIT III: ORGANIC SPECTROSCOPY-II

**Objective:** To have an idea about NMR spectroscopy

<sup>1</sup>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 – <sup>13</sup>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 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.

## **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.

### REFERENCES

- 1. Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, J. March, M.B. Smith, 6<sup>th</sup> Edn., Wiley, 2007.
- 2. Advanced Organic Chemistry, Part B: Reactions and Synthesis, F.A. Carey, R.A. Sundberg, 5<sup>th</sup> 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.
- 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	5 Hrs / Sem.: 75 Hrs / Unit: 15 Cree			

## 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

## UNIT II: STATISTICAL MECHANICS-II

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

Molecular Basis of residual entropy – Boltzmann distribution lawcomparison – 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.

### **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 –  $C_{2v}$ ,  $C_{3v}$ , $C_{2h}$ , $D_{3h}$ 

#### **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<sub>2</sub>O-NH<sub>3</sub>,BF<sub>3</sub>-Direct product of irreducible representation- selection rule for the  $n-\pi^*\& \pi-\pi^*$  transition in HCHO construction of Hybrid orbitals-CH<sub>4</sub>, [PtCl<sub>4</sub>]<sup>2</sup>-secular equation in MO theory-trans 1,3-butadiene, Benzene.

#### **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.

- 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, 4<sup>th</sup> 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, 3<sup>rd</sup> Edn., Oxford University Press, 1996.
- 6. Molecular Modeling, Principles and Applications, Second Edition, Andrew R Leech, Prentice Hall, NY, 2001.
- Guide Book on molecular modeling in Drug Design, N. Claude Cohen, 1<sup>st</sup> 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				
N <mark>ME</mark>	CHEMINFORMATICS 15PCHN31			
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 & Toxicityprediction 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 Non-Major elective				
NME	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.

Text Book of Pharmaceutical Chemistry – Jaysgree Ghosh, 2003;
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.

IV SEMESTER				
C10 ORGANIC CHEMISTRY - IV 15PCHC4				
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 interconversions, 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, a- 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, 5<sup>th</sup> Edn., 2000

3. Medicinal Chemsitry, Ashutosh Kar, 2<sup>nd</sup> 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, 1<sup>st</sup> 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				
C11	PHYSICAL CHEMISTRY - IV 15PCHC42			
Hrs / Week: 5	Hrs / Sem.: 75	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<sup>2</sup>, sp<sup>3</sup> 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  $\Delta$ H,  $\Delta$ G,  $\Delta$ S 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.

- 1. Quantum Chemistry, Donald A. Mcquire, Viva Books. 2011
- 2. Quantum Chemistry, A.B. Samigrahi, Books and Allied PVT Ltd, 2010.
- Introductory Quantum Chemistry, A.K. Chandra, 4<sup>th</sup> Edn., 2001, Tata McGraw Hill.
- 4. Quantum Chemistry IRA N. Levin, 6<sup>th</sup> Edn., PHI Learning PVT Ltd., New Delhi. 2009.
- 5. Molecular Quantum Mechanics, Atkins P W and R S Friedman, 3<sup>rd</sup> 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				
C12-P	PRO	15PCHP41		
Hrs / Week : 8	Hrs / Sem : 75	Hrs / Unit : 15	Credit : 6	

#### **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	<mark>5</mark>
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	A MEDICINAL CHEMISTRY 15PCH			
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 -  $\beta$ -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 drugspyrazinamide – 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

- 1. Organic Chemistry, I.L. Finar, Vol II, ELBS, 1975.
- Burger's Medicinal Chemistry and Drug Discovery Vol. I, 5<sup>th</sup>Edn. 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
- Drug Designs A Series of Monographs in Medicinal Chemistry, Edited by A. J. Ariens. I<sup>st</sup> 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 15PCHE				
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)

- 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
- 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
- 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 15PCH0				
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)
- <mark>ii. Ni(dmg)</mark>2
- iii. Potassium ferrioxalate
- iv. Cis- Chromiumdioxalatodihydrate
- v. Tri(acetylacetonato)manganese(III) Mn(acac)<sub>2</sub>
- vi. Prussian blue
- vii. Tetrammminecopper(II) sulphate
- viii. hexaamine cobalt(III) chloride

- 1) Vogel's Qualitative Inorganic Analysis, 7<sup>th</sup> 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 15PCHC4I				
Hrs / Week: 3 Hrs / Sem.: 60 Hrs / Year: 120 Cre				

# 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<sub>f</sub> values by
- 3. Identification of amino acid with the help of TLC or PC.
- Calculation of R<sub>f</sub> value of individual amino acid
- 4. Identification of sugar (glucose, fructose, sucrose) with the help of TLC or PC. Calculation of R<sub>f</sub> value.

- 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, 2<sup>nd</sup> Edn., New York: McGraw-Hill, 1987.
- 8. Practical Organic Chemistry, F G Mann and B C Saunders, 4<sup>th</sup> Edn., Pearson Education Ltd., 2009.
- 9. Textbook Of Practical Organic Chemistry, A I Vogel, Prentice Hall; 5<sup>th</sup> 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 15PCHC4P				
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<sub>4</sub> / 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:**

<u>www.gaussian.com</u>

# 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 CIA SEMESTER MARKS TEST EXAMINATION		SEMESTER	PASSING MINIMUM		
SUBJECT			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

# SUBJECTMARKSASSIGNMENT<br/>OR SEMINAR<br/>FOR PGREGULARITYRECORD<br/>NOTETOTAL<br/>MARKSTheory205--25

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Practical

30

# **DIVISION OF MARKS FOR CIA TEST**

1. The duration of each CIA Test is ONE hour and the Semester Examination is THREE hours.

5

5

40

- 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:

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
Α	No Choice Answer should not exceed 75 words	2 Questions 2 marks each	2 x 2 = 4
В	Internal choice (Either or type) Answer should not exceed 200 words	2 Questions 4 marks each	2 x 4 = 8
С	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
в	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
с	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
	75 MARKS		