Sadakathullah Appa College

(Autonomous)

(Reaccredited by NAAC at an 'A' Grade and ISO 9001:2015 Certified Institution)

Rahmath Nagar, Tirunelveli – 627 011, Tamil Nadu.

PG DEPARTMENT OF CHEMISTRY

CBCS SYLLABUS

For

M.Sc. Chemistry

(Applicable for students admitted in June 2019 and onwards)
(As per the Resolutions of the Academic Council Meetings held on 03-03-2018, 17-10-2018 and 02-03-2019).

CONTENTS

POST GRADUATE DEPARTMENT OF CHEMISTRY
CBCS SYLLABUS M.Sc. CHEMISTRY (2018 - 2021)
COURSE STRUCTURE (CBCS)
(Applicable for students admitted in June 2019 and onwards)

I SEMESTER			**II SEMESTER**		
COURSE	**H/W**	**C**	**COURSE**	**H/W**	**C**
DSC 1	6	4	DSC 4	5	4
DSC 2	6	4	DSC 5	5	4
DSC 3	6	4	DSC 6	5	4
DSE 1	4	4	DSE 2	4	4
P-I	4	2	P-III	4	2
P-II	4	2	P-IV	4	2
			IDC-I	3	3
TOTAL	**30**	**20**	**TOTAL**	**30**	**23**
III SEMESTER			**IV SEMESTER**		
DSC 7	5	4	DSC 10	5	4
DSC 8	5	4	DSC 11	5	4
DSC 9	5	4	DSC 12- Project	8	8
DSE 3	4	4	DSE 4	4	4
P-V	4	2	P-VII	4	2
P-VI	4	2			
			P-VIII	4	2
IDC 2	3	3			
TOTAL	**30**	**23**	**TOTAL**	**30**	**24**
I – IV SEMESTER					
MOOC*		2#			

DISTRIBUTION OF HOURS, CREDITS, NO. OF PAPERS, & MARKS				
SUBJECT	**HOURS**	**CREDITS**	**NO. OF PAPERS**	**MARKS**
DSC THEORY + PROJECT	66	52	12	1200
DSC PRACTICALS	32	16	8	400
DSE	16	16	4	400
IDC	6	6	2	200
MOOC*		2#	1	
TOTAL	**120**	**90+2#**	**27**	**2200**

COURSE STRUCTURE
POSTGRADUATE AND RESEARCH DEPARTMENT OF CHEMISTRY
CBCS Syllabus – M.Sc., Chemistry (2019 - 2020 onwards)

Sem	P	Title of the Paper	Sub. Code	H/W	C	Marks		
						I	E	T
I	DSC1	INORGANIC CHEMISTRY – I	18PCCH11	6	4	25	75	100
	DSC2	ORGANIC CHEMISTRY – I	18PCCH12	6	4	25	75	100
	DSC3	PHYSICAL CHEMISTRY – I	18PCCH13	6	4	25	75	100
	DSE1A	CHROMATOGRAPHY	18PECH1A	4	4	25	75	100
	DSE1B	BIOCHEMISTRY	18PECH1B					
	P-I	INORGANIC CHEMISTRY PRACTICALS -I	18PCCH1P1	4	2	40	60	100/2
	P-II	PHYSICAL CHEMISTRY PRACTICALS - I	18PCCH1P2	4	2	40	60	100/2
II	DSC4	INORGANIC CHEMISTRY - II	18PCCH21	5	4	25	75	100
	DSC5	ORGANIC CHEMISTRY – II	18PCCH22	5	4	25	75	100
	DSC6	PHYSICAL CHEMISTRY – II	18PCCH23	5	4	25	75	100
	DSE2A	APPLIED CHEMISTRY	18PECH2A	4	4	25	75	100
	DSE2B	CHEMINFORMATICS	18PECH2B					
	P-III	ORGANIC CHEMISTRY PRACTICALS – I	18PCCH2P1	4	2	40	60	100/2
	P-IV	CHROMATOGRAPHY PRACTICALS	18PCCH2P2	4	2	40	60	100/2
	IDC-1	INDUSTRIAL CHEMISTRY	18PICH21	3	3	25	75	100
III	DSC7	INORGANIC CHEMISTRY - III	18PCCH31	5	4	25	75	100
	DSC8	ORGANIC CHEMISTRY – III	18PCCH32	5	4	25	75	100
	DSC9	PHYSICAL CHEMISTRY – III	18PCCH33	5	4	25	75	100
	DSE3A	INSTRUMENTAL METHODS OF ANALYSIS	18PECH3A	4	4	25	75	100
	DSE3B	ENZYME CHEMISTRY	18PECH3B					
	P-V	ORGANIC CHEMISTRYPRACTICALS - II	18PCCH3P1	4	2	40	60	100/2
	P-VI	PHYSICAL CHEMISTRY PRACTICALS-II	18PCCH3P2	4	2	40	60	100/2
	IDC-2	INTRODUCTION TO CHEMINFORMATICS	18PICH31	3	3	25	75	100
IV	DSC10	SPECTROSCOPY	18PCCH41	5	4	25	75	100
	DSC11	ADVANCED TOPICS IN CHEMISTRY	18PCCH42	5	4	25	75	100
	DSC12	PROJECT	18PCCH43	8	8			100
	DSE4A	MEDICINAL CHEMISTRY	18PECH4A	4	4	25	75	100
	DSE4B	RATIONAL DRUG DESIGN	18PECH4B					
	P-VII	INORGANIC CHEMISTRY PRACTICALS II	18PCCH4P1	4	2	40	60	100/2
	P-VIII	GREEN CHEMISTRY PRACTICALS	18PCCH4P2	4	2	40	60	100/2
I-IV		Massive Open Online Course *		-	2#			
Total				**120**	**90+2#**			**2200**

* As per the guidelines of the UGC all the UG and the PG students shall enroll for one Massive Open Online Course offered through SWAYAM, NPTEL, etc.
# Two extra credits will be given on completion of the course.

I SEMESTER			
DSC1	**INORGANIC CHEMISTRY – I**		**18PCCH11**
Hrs / Week: 6	**Hrs / Sem.: 90**	**Hrs / Unit: 18**	**Credit: 4**

UNIT I: SOLID STATE CHEMISTRY

Description of crystal structure – NaCl, Zinc blende (Sphalerite and Wurtzite), Fluorite, Antifluorite, Perovskite, $CdCl_2$,CsCl, K_2NiF_4, Spinel, Inverse Spinel and Rutile.

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, INORGANIC CHAINS, RINGS, AND CAGES.

VSEPR theory – Postulates and applications of VSEPR theory– Bent's rule – Apicophilicity of dπ-pπ bonds

M.O theory – symmetry and overlap – M.O diagram of HF and BeH_2, Walsh diagram (triatomic molecules- BeH_2 and CO_2).

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

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

Cages – Preparation and structure of phosphorous cage molecules, Diboranes, Styx number, tetraboranes. Structures of B_5H_9, B_5H_{11},B_6H_{10}, $[B_8H_8]^{2-}$, Structural relationships of closo, nido and arachno boranes.

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 IIII: STEREOCHEMISTRY & COORDINATION CHEMISTRY-I

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: COORDINATION CHEMISTRY II

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: COORDINATION CHEMISTRY III

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, Prentice-Hall, 1967.
3. Solid State Chemistry D. K. Chakrabarty, New Age International, 2010.
4. Inorganic Chemistry - Principles, structure and reactivity, IV edition, James E. Huheey, Ellen A Keitier, Richard LKeiter Pearson Publication (2012).
5. Concise Inorganic Chemistry, J. D. Lee, Elbs with Chapman and Hall, London.
6. Advanced Inorganic Chemistry, F. A. Cotton, R. G. Wilkinson, 6thEdn., Wiley, 1996.
7. Inorganic Chemistry, D.F. Shriver and P.W. Atkins, 4thEdn., Harper Collins, 1993.
8. Modern Inorganic Chemistry, R. D. Madan & Satya Prakash, S Chand and Company, Ltd., 1st Edn., 1987.
9. Principles of Inorganic Chemistry, Puri, Sharma and Kalia, 31st edition, Milestone Publishers.
10. Modern Inorganic Chemistry, Willam L. Jooly, Magraw-Hill, 1991.
11. Inorganic Chemistry, Gary L. Miessle and Donald A. Tarr, Dorling Kindersley (India) Pvt. Ltd., 3rdEdn., 2009.

I SEMESTER			
DSC 2	**ORGANIC CHEMISTRY – I**		**18PCCH12**
Hrs / Week: 6	**Hrs / Sem.: 90**	**Hrs / Unit: 18**	**Credit: 4**

UNIT I: REACTIVE INTERMEDIATES, ENAMINES AND YLIDES:

Reaction intermediates:

Carbocation: Formation, Reactions, Stability, Structure.

Non-Classical Carbocations: Neighbouring group participation (C-C, C=C, Cyclopropyl, Aromatic rings as neighbouring group).

Carbanion- Formation, Reactions, Stability, Structure, effect of substituents on resonance stabilized carbanions.

Free radicals – Formation, Reactions, Stability, Structure.

Carbenes: Types of carbene, Formation, Reactions, Stability, Structure.

Arynes- Formation, Reactions, Stability, Structure, trapping method.
Nitrenes- Generation, Reactions, Structure.

Enamines: Formation and reactions.

Ylides – Generation and reactions.

UNIT II: REAGENTS IN OXIDATION AND REDUCTION IN ORGANIC SYNTHESIS:

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

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 tetraacetate, Grignard Reagent.

UNIT IV: 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: 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. Organic Chemistry, Volume I, S.M. Mukherji, S.P. Singh, R.P. Kapoor and R. Dass, 2nd edition, New Age International Publishers.
2. March's Advanced Organic Chemistry, Reactions, Mechanisms and Structure, Jerry March, Michael B. Smith, 6thEdn., A John Wiley& Sons Ltd, 2007.
3. Organic Reaction and Mechanisms, V.K. Ahluwalia, Rakesh Kumar Parashar, 3rd edition.
4. Nomenclature of Organic compounds: Principles and Practice, Robert B. Fox and Warren H. Powell, 2nd edition, American Chemical Society, Oxford University Press.
5. Advanced Organic Chemistry, Part A: Structure and Mechanisms, F.A. Carey, R.A. Sundberg, 5th Edn., Springer, 2007.
6. Organic Reaction Mechanisms, A.C. Knipe, John Wiley& Sons Ltd. Publications, 2012.
7. Synthetic Approaches in Organic Chemistry, Raj K. Bansal, Jones and Barlett Publishers, International, 1998.
8. Advanced Organic Chemistry: Reaction Mechanisms, R. Bruckner, Academic Press, 2002.
9. Organic Chemistry, J. Clayden, N. Greeves, S. Warren, P. Wothers,Oxford University Press, 2004.
10. Mechanism and Theory in Organic Chemistry, T.H. Lowry, K.S. Richardson,2nd Edn.Harper& Row, 1981.
11. Stereochemistry of Organic Compounds: Principles and Applications, D. Nasipuri, 3rd Edn., New Age Pub., 2010.
12. Organic Reaction Mechanisms, V.K. Ahluwalia and Rakesh Kumar Parashar,Narosoa Publishing House, 4th Edn., 2011.
13. Jie Jack Li, Gordon W. Gribble Palladium in Heterocyclic Chemistry, 2nd Edn., Tetrahedron Organic Chemistry Series, Volume 26, Elsevier, 2006.
14. Modern synthetic reactions, Herbert O. House, Benjamin-Cummings Publishing Co., 1972.
15. Organic Synthesis, Michael B. Smith, 2nd Edn., McGraw-Hill Higher Education, 2002.

I SEMESTER			
DSC 3	**PHYSICAL CHEMISTRY – I**		**18PCCH13**
Hrs / Week: 6	**Hrs / Sem.: 90**	**Hrs / Unit: 18**	**Credit: 4**

UNIT I CHEMICAL 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 IRREVERSIBLE 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 nonlinear systems.

UNIT III 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- QUANTUM CHEMISTRY-I

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-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.
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, III Edition, Pearson.
7. Physical Chemistry, Alberty, R.A., and R.S. Silbey and M.G. Bawendi, 4th Edn., Wiley, 2005.
8. A textbook 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.
11. Quantum Chemistry, Donald A. Mcquire, Viva Books, 2011.
12. Quantum Chemistry, A.B. Samigrahi, Books and Allied Pvt. Ltd, 2010.
13. Introductory Quantum Chemistry, A.K. Chandra, 4th Edn., Tata McGraw Hill, 2001.
14. Quantum Chemistry, Ira N. Levin, Edition VI, PHI Learning PVT Ltd., New Delhi, 2009.

I SEMESTER			
DSE1A	**CHROMATOGRAPHY**		**18PECH1A**
Hrs / Week: 4	**Hrs / Sem.: 60**	**Hrs / Unit: 12**	**Credit: 4**

UNIT I: CHROMATOGRAPHY-INTRODUCTION

Classification- Chromatographic methods, Column Chromatography- Principles, Experimental procedures, stationary and mobile phases, Choice of solvent systems, Separation techniques, Applications.

R_f 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

Principles, factors affecting R_f 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

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

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

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			
DSE1B	**BIOCHEMISTRY**		**18PECH1B**
Hrs / Week: 4	**Hrs / Sem.: 60**	**Hrs / Unit: 12**	**Credit: 4**

UNIT I: CARBOHYDRATES

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**

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

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

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

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, LehingerJ.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 — LubertStryer – W. H. Freeman and company, 4th Edn., New York, 1995.
7. Biochemistry, S.C. Rastogi, Ane Book (Pvt.) Ltd., 2nd Edn., 2003.
8. Biochemistry, Keshav Trehan, New Age International, 2nd Edn., 1990.
9. 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
8. Estimation of $KMnO_4$
9. Estimation of strengths of strong and weak acid in a mixture
10. Determination of dissociation constant of a weak acid

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			
DSC 4	**INORGANIC CHEMISTRY - II**		**18PCCH21**
Hrs / Week: 5	**Hrs / Sem.: 75**	**Hrs / Unit: 15**	**Credit: 4**

UNIT I: 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: 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: 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 ($Fe(CO)_2(NO)_2$, $Co(CO)_3(NO)$, $Mn(CO)_4(NO)$, (η^5-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: 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: 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. Tuliand 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, SleptrenCredock, Blackwell; 2nd Edn., 1991.
12. Physical Inorganic Chemistry- A Coordination Approach, S.F.A.Kettel, Oxford University Press; New edition, 1998.
13. Inorganic Chemistry - Principles, structure and reactivity, IV edition, James E. Huheey, Ellen A Keitier, Richard L Keiter Pearson Publication (2012).
14. Inorganic Chemistry - Principles, structure and reactivity, J E Huheey, Harper and Row Publisher, Inc. New York (1972)
15. Concise Inorganic Chemistry, J. D. Lee, Elbs with Chapman and Hall, London.
16. Advanced Inorganic Chemistry, F. A. Cotton, R. G. Wilkinson, 6th Edn., Wiley, 1996.
17. Inorganic Chemistry, D.F.Shriver and P.W. Atkins, 4th Edn., Harper Collins, 1993.
18. Modern Inorganic Chemistry, R. D. Madan & Satya Prakash, S Chand and Company, Ltd., 1st Edn., 1987.
19. Essentials of Nuclear Chemistry, H.J. Arnikar, Wiley Eastern Ltd., India, 4th Edn., 2000.
20. Nuclear and Radiation Chemistry, G. Friedlander, J.W. Kennedy and N.M.Miller, John Wiley, 1981.

II SEMESTER			
DSC 5	**ORGANIC CHEMISTRY-II**		**18PCCH22**
Hrs / Week: 5	**Hrs / Sem.: 75**	**Hrs / Unit: 15**	**Credit: 4**

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UNIT I: STEREOCHEMISTRY

Chirality – prochirality – enantiotopic and diastereotopic atoms, Fischer, Wedge, Newmann and Sawhorse formulas, RS, EZ notation, Conformational analysis - dihedral angle-factors, Conformational analysis of 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: 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

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

UNIT IV: 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: 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.

REFERENCES:

1. Stereo Chemistry – Conformation and Mechanism, Kalsi, New Age International (P) Ltd 2000.
2. Stereo Chemistry Of Carbon Compounds, E L Elliel, McGraw Hill 1999.
3. Introduction to Stereochemistry, K. Mislow, W.A.Benjamin, New York, 1966.
4. Stereo Chemistry, V M Potapov, MIR publications 1979.
5. Advanced Organic Chemistry, 4th Edn., Jerry March, 1992
6. A Guidebook To Mechanism In Organic Chemistry, P. Sykes, Orient Longman, 1989.
7. Fundamentals Of Organic Reaction Mechanism, J M Harris and C Wamser, 1st Edn., John, Wiley and Sons, 1976.
8. Reaction Mechanism Inorganic Chemistry, S M Mukherji and S P Sing, Macmillan India Ltd., 2009.
9. Organic chemistry, Paula Yurkanis, 3rd Edn, Pearson Education Asia 2002.
10. Fundamentals of Photochemistry – K.K.Rohatgi – Mukherjee (Revised Edition) New age International publications, Reprint 2002.
11. Molecular Photochemistry N.J.Turro and W.A. Benjamin.
12. Molecular reactions and Photochemistry - Charles H.Depuy, Orville.S. Chapman, Prentice – Hall of India Pvt., Ltd. 1988.
13. Photochemistry in Organic Synthesis, J.D. Coyle – Royal society of Chemistry, 1986.
14. Organic Chemistry, Volume II, Stereochemistry and the Chemistry of Natural Products, I.L. Finar, 5th Edn, 2000.
15. Heterocyclic Chemistry, J. A. Joule, K. Mills and G.F. Smith, 3rd Edition, Stanely Thornes Publishers Ltd,2004.

II SEMESTER			
DSC 6	**PHYSICAL CHEMISTRY – II**		**18PCCH23**
Hrs / Week: 5	**Hrs / Sem.: 75**	**Hrs / Unit: 15**	**Credit: 4**

UNIT I – 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

Debye – Huckel theory of strong electrolytes –derivation and verification– Activity coefficient of electrolytes – activity coefficient – ionic strength – 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

Kinetics of electrode reaction – Butler 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: 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 Orthogonality Theorem (GOT) – Use of GOT to construct character tables – character tables for point groups – C_{2v}, C_{3v},C_{2h},D_{3h}.

UNIT V: 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. Principles of Physical Chemistry, Puri, Sharma and Pathania, Vishal Publications, 46th Edition, 2008.
2. Principles and Applications of Electrochemistry, Crow, D.R., Chapman and Hall, 1988.
3. Electrochemistry, Reiger, P.H., Chapman and Hall, 2nd Edn., 1983.
4. Group Theory in Chemistry, Gopinathan, M.S., and V. Ramakrishnan, Vishal Publications, Jalandhar (India), 1986.
5. Group Theory and Applications in Chemistry, Raman, K.V., Tata McGraw-Hill, New Delhi, 1990.
6. Group Theory and Symmetry in Chemistry, Hall, L.H., McGraw-Hill, 1969.
7. Group Theory and Applications to Quantum Mechanics of Atomic Spectra, Academic Press, 1959.
8. Physical Chemistry, Peter Atkins and Julio de Paula, W. H. Freeman and Company, 8th edition, 2006.

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, Fermentation processes, Manufacture of spirits, Manufacture - vinegar, power alcohol, Ethyl alcohol from molasses, preparation of wash, Distillation, Alcohol from waste sulphite liquor, Manufacture from - starchy materials, cellulose materials, 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 - cotton seed oil by expression and solvent extraction, 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, Zinc oxide, Titanium dioxide, red lead - characteristics of the pigment, Uses - Blue pigments, ultramarine blue, cobalt blues and iron blues, red pigments, synthetic iron oxide pigment, green pigments, chrome green, black pigments, yellow pigments – Tonners - Metallic powders as pigments.

Paints: Classification, Constituents, Requirements of a good paint, Importance of PVC, paint failure, Emulsion paints - Constituents, Advantages, Latex paints, Luminescent paints, Fire retardant paints, Heat resistant paints.

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) Textbook 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			
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 – 3D 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.

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 tribromoaniline from aniline.

REFERENCES:

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 Textbook 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 by TLC
2. Benzophenone and benzoic acid and checking their R_f values by TLC
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 Handbook 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			
DSC7	**INORGANIC CHEMISTRY - III**		**18PCCH31**
Hrs / Week: 5	**Hrs / Sem.: 75**	**Hrs / Unit: 15**	**Credit: 4**

UNIT I: ORGANOMETALLIC CHEMISTRY – I

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, Zeisel's salt, acetylene and π-allyl complexes.

UNIT II: ORGANOMETALLIC CHEMISTRY – II

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's Natta Catalyst), Cyclooligomerization of olefins and acetylenes using Ni catalyst (Reppe's catalyst).

UNIT III: BIOINORGANIC CHEMISTRY - I

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

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: ORGANOMETALLIC CHEMISTRY – III

Transition metal – hydrogen compounds. General synthetic methods, Chemical behaviour, 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, 4thEdn., 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. Tuliand 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.

III SEMESTER			
DSC8	**ORGANIC CHEMISTRY - III**		**18PCCH32**
Hrs / Week: 5	**Hrs / Sem.: 75**	**Hrs / Unit: 15**	**Credit: 4**

UNIT I: PERICYCLIC REACTIONS

Dienophile, diene, Cyclic dienes, Heterodienes - Regiochemistry and Stereochemistry of the Diels–Alder Reaction - Intramolecular - The retro - 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 - [2,3]-Sigmatropic rearrangements - Electrocyclic reactions.

UNIT II: ALKALOIDS

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

Biogenesis of alkaloids

UNIT III: 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, zingiberene and abietic acid.

UNIT IV: 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: 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. 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. Chemistry of Natural Products, S.V. Bhat, B.A. Nagasampagi, N. Sivakumar, Narosa Publishing House, New Delhi, 2010.
6. Organic Chemistry, I L Finar, Vol II ELBS, 5th Edn., 2000
7. Medicinal Chemsitry, Ashutosh Kar, 2nd Edn., New Age International (Pvt.) Publishers, 2007.
8. Organic Chemistry of Natural Products, Volume II, Chatwal Gurdeep R, Himalaya Publishing House, 2009.
9. S. Sankararaman, Pericyclic Reactions-A Textbook, Wiley VCH, 2005.
10. Organic Chemistry, J. Clayden, N. Greeves, S. Warren, P. Wothers, Oxford University Press, 2004.
11. Organic Chemistry, Volume II, Stereochemistry and the Chemistry of Natural Products, I.L. Finar, Longmans, 1964.

III SEMESTER			
DSC9	**PHYSICAL CHEMISTRY - III**		**18PCCH33**
Hrs / Week: 5	**Hrs / Sem.: 75**	**Hrs / Unit: 15**	**Credit: 4**

UNIT I: 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 THERMODYNAMICS-I

Modern Theoretical principles: 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: 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. Fermi energy - Electron gas in metals.

UNIT IV: 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: 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. 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. Elements of statistical thermodynamics - L. K. Nash, Addison Wesley
4. Statistical thermodynamics by B. J. McCelland, Chapman and Hall.
5. A Introduction to Statistical Thermodynamics by T. L. Hall Addison - Wesley
6. Advanced physical Chemistry by S. N. Blinder, The Macmilan Company, 1967.
7. Themodynamics by R. C. Srivatsava, S. Saha and A. K. Jain, Prentice-hall, India.
8. Physical Chemistry, Kundu N, and Jain S.K., S. Chand and Co., New Delhi, 1984.
9. Quantum Chemistry, Donald A. Mcquire, Viva Books, 2011.
10. Quantum Chemistry, A.B. Sanigrahi, Books and Allied Pvt. Ltd, 2010.
11. Introductory Quantum Chemistry, A.K. Chandra, 4th Edn., Tata McGraw Hill, 2001.
12. Quantum Chemistry, Ira N. Levin, Edition VI, PHI Learning PVT Ltd., New Delhi, 2009.
13. Principles of Physical Chemistry, Puri, Sharma and Pathania, 46th Edition, Vishal Publications, 2008.

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.

UNITII - 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, 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, Instrumentation and 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			
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.
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.

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			
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 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 organometallic 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, 6thEdn., Wiley, 2007.
2. Advanced Organic Chemistry, Part B: Reactions and Synthesis, F.A. Carey, R.A. Sundberg, 5thEdn., 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			
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 challenges 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 geneome 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		
DSC12	**PROJECT**	**18PCCH43**
Hrs / Week : 8	**Hrs / Sem : 120**	**Credit : 8**

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 be formed as 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			
DSE4A	**MEDICINAL CHEMISTRY**		**18PECH4A**
Hrs / Week: 4	**Hrs / Sem.: 60**	**Hrs / Unit: 12**	**Credit: 4**

UNIT I: 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, 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, 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, Ashutosh Kar, New Age International Publishers, 2007.
11. The Organic Chemistry of Drug Design and Drug action R. Silverman, (Ed) Academic Press, 2004.

IV SEMESTER			
DSE4B	**RATIONAL DRUG DESIGN**		**18PECH4B**
Hrs / Week: 4	**Hrs / Sem.: 60**	**Hrs / Unit: 12**	**Credit: 4**

UNIT I: INTRODUCTION

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

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

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

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

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. Textbook 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.

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 (G) and calcium (V)

II Preparation of Inorganic Complexes

i. Tris -acetylacetonato iron(III)
ii. $Ni(dmg)_2$
iii. Potassium ferrioxalate
iv. Cis- Chromium dioxalatodihydrate
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. Bioinformatics – a practical guide to the analysis of Genes and Proteins, Baxevanis, A.D. and Francis Ouellellette, , John Wiley & Sons, UK, 1998.
5. Molecular Modeling, Principles and Applications, II Edition, Andrew R. Leach, Dorset Press, Dorchester, Dorset, 2001.
6. Lednicer, D.(1998). Strategies for Organic Drug Discovery Synthesis and Design.Wiley International Publishers.