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DEPARTMENT OF CHEMISTRY

(Effective for those admitted from 2017-2018 onwards)



SYLLABI

M.Sc., CHEMISTRY

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M.Sc., CHEMISTRY

(Effective for those admitted from 2017-2018 onwards)

SEMESTER – I

CC 1 - ORGANIC CHEMISTRY I

Subject Code: 17P1C1	Credits: 5	External Marks: 75	Hours: 6

- **UNIT I: Nomenclature:** IUPAC nomenclature of complex organic molecules acyclic compounds mono, bi and tricyclic compounds polynuclear hydrocarbons heterocycles- five membered, six membered, five and six membered fused heterocycles rare alkaloids such as indoloquinolines, naphthyridines and fused carbazoles. Reaction intermediate: formation, stability, detection and reactions of carbonium ions carbanions- carbon radical carbenes nitrenes.
- **UNIT II: Aromaticity:** Six membered ring five, seven and eight membered rings other system containing aromatic sextet alternate and non alternate hydrocarbons aromatic system with electron numbers other than six systems of two electrons. Systems of four electrons anti aromaticity systems of eight electrons, ten electrons and more than ten electrons: 4n+2 electrons other aromatic compounds meso ionic compounds, the dianion of squaric acid and homo aromatic compounds.
- UNIT III: Addition and Elimination: Addition to double and triple bonds Mechanism Hydration Hydroboration Hydroxiylation epoxidation. Elimination reactions E1, E2, E1cB Mechanism Orientation effects in elimination reactions stereo chemistry of elimination reactions dehydration of alcohols dehydro halogenation cope elimination.

UNIT IV: Aliphatic Electrophilic Substitution Reactions: Mechanisms-

Bimolecular mechanisms- SE2 and SEi - SE1 mechanism-electrophilic substitution accompanied by double bond shifts-other mechanisms. Reactivity - Effect of substrate - effect of leaving group and effect of solvents.Reactions - hydrogen as a leaving group-migration of double bonds ketoenoltautomerism. Halogen electrophiles - halogenation of aldehydes and ketones, halogenation of carboxylic acids and acyl halides- halogenation of sulfoxides and sulfones- nitrogen electrophiles-sulfur electrophiles- carbon electrophiles- Stork enamine reaction.

UNIT V: Aromatic electrophilic substitution Reactions: Mechanisms- arenium ion mechanism-effects on arenium ion mechanism including isotope effect – isolation of arenium ion intermediate - SE1 mechanism. Orientation and reactivity - orientation and reactivity in mono substituted benzene rings – orthopara ratio - ipso attack – orientation in benzene ring with more than one substituent – orientation in other ring systems- quantitative treatments of reactivity in the substrate – the effect leaving group -mechanism of following reactions - nitration – sulphonation – halogenation - Friedel Crafts reaction – Scholl reaction - Gattermann Koch reaction - HoubenHoesch synthesis – Vilsmeier Haack reaction- Gattermann reaction- Reimer-Tiemann reaction-Kolbe Schmitt reaction.

References:

- 1. Advanced Organic Chemistry; Reactions, Mechanisms and Structure -Jerry March.
- 2. Reaction Mechanism in Organic Chemistry S. M. Mukherji and S. P. Singh.
- 3. Advanced Organic Chemistry; Part A Structure and Mechanisms, -Carey and Sundberg.

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SEMESTER – I

CC 2 - INORGANIC CHEMISTRY I

Subject Co	de: 17P1C2	Credits: 5	External Marks: 75	Hours: 6
UNIT I:	Defects-Stoichio excess and met conductor, insu High Tc, Magn	al deficiencies. Electr ilator, semiconducto etic properties- para	olids layer and vacancies- Non ical properties- band theory r (n and p), superconducto , dia, ferro, antiferro and escence, laser and inorganic	y, VB and MO theory, or-types, BCS theory, ferri magnetism and
UNIT II:	Acid-Base and Usanovich conc base strength – – theoretical b	Non-aqueous Solven eept of acid and base E and C parameters asis for hardness a	n ts – steric and salvation effect . Hard and Soft Acids and I	ts – measure of acid – Bases (HSAB concept) us solvents: Liq.NH ₃ ,
UNIT III:	Borozine – boro of silicones-Ty phosphonitrilic	ners – classification - oxine -BN (Boron nitr /pes of silicones. chloride-poly ortho	general properties - polyme ide). Silicones - preparation Polymers containing pl ophosphoric acids-polyme cates-Type-preparation, pro	ns – properties - uses hosphorus-Types-poly ric compounds of
UNIT IV:	by Aston and D methods-fractio capture reactio plant-Nuclear determination counter. Partic	pe-detection and mea empster's mass spec- on evaporation meth n, fission reaction, structure-liquid dro of activity by cloud le accelerators- linea	asurement by GM counter. I troscopy-separation of isoto od. Nuclear reactions-Tra spallation reaction. Nuclea op model and shell mo l chamber, bubble cham ar accelerator, cyclotron a and medicinal chemistry.	opes-thermal diffusion nsmutation reaction, ar reactor and power odel. Detection and ber and scintillation
UNIT V:	potassium pun anhydrase an	piology- Mechanism o np, Photosynthesis - d Carboxypeptidase riedoxin, nitrogen fix	of ion transport across me PSI, PSII, Porphyrins, Met , Oxygen transport, Irc ation, metal complexes in r	alloenzymes-Carbonic on-sulphur proteins-
Reference	Concepts and n	rn aspects of inorgan	nemistry B.E. Douglas, D.H. ic chemistry, H.J.Emeleus,	
2. 3. 4. 5. 6. 7.	Advanced Inorgan New concise Inorgan Inorganic chemiss Inorganic chemiss Source Book on A Essentials of nucc Nuclear and radii Wiley – Interscien	nic Chemistry: A Com ganic chemistry, J. D try, K. F. Purcell & J. try: Principles of stru atomic Energy, Samu- lear chemistry, H.J.A ochemistry, G.Friedla	prehensive Text, F.A. Cotto . Lee, Van Nostrand – Reinh C. Kotz, Saunders, Philade cture and reactivity, J. E. H el Glasstone, D. Van Nostra rnikar, Wiley Eastern Ltd., ander, J.W.Kennedy, E.S.M ements in the Chemistry of	nold, New York, 1964 Iphia, 1977 Iuheey. Ind – Reinhold 1987 Iacias and J.M.Miller,

- Schewederski, , John Wiley & Sons, New York, USA.
- 9. Bioinorganic Chemistry, R. W. Hay.
- 10. Principles of Bioinorganic Chemistry, S.J. Lippard and J. M. Berg, , Panima Publishing Company, New Delhi, 1997.

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SEMESTER – I

CC 3 - INDUSTRIAL & AGRICULTURE CHEMISTRY

	Subjec	t Code: 17P1C3	Credits: 4	External Marks: 75	Hours: 6		
U	NIT I:	Fuels: Introduction	n – classification of	fuels - calorific value - char	cacteristics of an		
		ideal fuel. Solid	fuel: classification	of coal -proximate and ul	timate analysis–		
		carbonization of co	oal. Liquid fuel: cruc	1e petroleum – cracking – typ	es – properties –		
		knocking - octane	and cetane numbers	s – anti-knocking – flash point	t – smoke point –		
		production of synthetic petrol – Fischer-Tropsch method, Bergius method. Fuel					
		gases: Manufacture and industrial applications of coal gas, producer gas, water gas,					
		semi-water gas and	d LPG.				

- UNIT II: Paints constituents manufacture requirements emulsion paint varnishes.
 Pigments- classification -Examples. Dyes -classification based on structure and application azo dyes xanthene dyes. Paper and pulp manufacture of pulp mechanical, chemical and semi chemical methods -Production and types of paper.
 Soaps classification, manufacture cleaning action of soap detergents principal groups of synthetic detergents -comparison of soaps and detergents.
- UNIT III: Basic Concepts of polymer science: Classification of polymers Types of polymerization techniques. Polymer degradation -Types of degradation –Polymer reactions- Hydrolysis, hydrogenation, addition and substitution reactions –cross-linking reactions. Experimental methods: Polymer synthesis, isolation and purification of polymers fractionation Fiber science: Natural fibers cotton, wool, silk general characteristics synthetic fibers poly amide fiber Nylon 66 preparation, properties.
- UNIT IV: Soil chemistry: Chemical composition of soil mineral and organic constituents properties adsorption and desorption soil reactions. Soil Physics: Physical composition of soil Soil air, Soil temperature, Soil water, Soil moisture contents. Soil fertility: Concept of nutrient availability soil fertility evaluation principles and methods of soil test crop response studies. Fertilizer recommendations. Nutrition requirements: Characteristics of essential element role of essential elements in plant nutrition nutrient deficiency symptoms secondary nutrients and micro nutrients-their function in plants.
- UNIT V: Chemistry of Fertilizers: Requirements of good fertilizer classification.
 Fertilizers: Effect of nitrogen, potassium and phosphorous on plant growth manufacture and composition of urea, triple super phosphate, complex fertilizers, mixed fertilizers and biofertilizers. Pesticides: classification general methods of preparation and applications toxicity safety measures. Insecticides: Insecticides: Nicotine, pyrithrin, borates, DDT and BHC. Fungicides: Bordeaux mixture MCO. Herbicides: MCPA, MCPB and MCPP.

References: Industrial Chemistry, B. K. Sharma.

B.N.Chakrabarthy, Industrial Chemistry, Oxford and IBH, New Delhi, 1981

- 1. Polymer Science, V.R. Gowariker et al., Wiley Eastern, 1986.
- 2. Fundamentals of Polymer Science and Engineering, Kumar Gupta, Tata McGraw Hill, 1981.
- 3. Textbook of Soil Science T.D. Biswas, S.K. Mukherjee, Tata McGraw Hill (1994).
- 4. Agricultural Chemistry, Vols. 1 and 2, Edited by Yagodin, Mir Publishers, Mascow.
- 5. Fundamentals of Soil Science C.E.Millar, L.M.Turk, H.D.Foth, John Wiley and Sons, (1965).
- 6. Soil Fertility in India, R.R.Ararwal, Asia Publishing Hosue. (1967) Soil Physics L.D.Baver, Asia Publishing Hosue. (1960).

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SEMESTER – I CC - PRACTICAL I INORGANIC CHEMISTRY I

Semi-micro qualitative analysis

Analysis of a mixture contains four basic radicals of which two common and two rare earths.

Common Basic radicals

Lead, Copper, Cadmium, Bismuth, Aluminium, Iron, Zinc, Nickel, Calcium, Magnesium and Barium

Rare-earths

Tellurium, Cerium, Selenium, Tungsten, Molybdenum, Thorium, Zirconium, Vanadium and Lithium

Calorimetric Estimations

- 1. Estimation of Nickel
- 2. Estimation of Copper
- 3. Estimation of Iron

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SEMESTER – I CC - PRACTICAL II PHYSICAL CHEMISTRY I

Potentiometric Titrations

- 1. Strong acid Vs Strong Base
- 2. Weak acid Vs Strong Base
- 3. Mixture of acids Vs Strong Base
- 4. Redox Titrations
- 5. Titration between KCl Vs $AgNO_3$
- 6. Mixture of halides Vs AgNO₃
- 7. Determination of pH of Buffer solution
- 8. Solubility of a sparingly soluble salt

Conductometric Analysis

- 1. Strong acid Vs Strong Base
- 2. Weak acid Vs Strong Base
- 3. Mixture of acids Vs Strong Base
- 4. Strong acids Vs Weak Base
- 5. Determination of cell constant
- 6. Verification of Debye-Huckel-Onsagar Equation
- 7. Verification of Oswalds Dilution Law
- 8. Determination of solubility of Lead sulphate in Water
- 9. Precipitation Titration

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SEMESTER – II

CC 4 - ORGANIC CHEMISTRY II

Subject Co	de: 17P2C4	Credits: 5	External Marks: 75	Hours: 6
UNIT I:	Aliphatic nucle	ophilic substitution re	actions: Mechanisms - the SN	12

- mechanism the SN1 mechanism ion pairs in the SN1 mechanism mixed SN1 and SN2 mechanisms - SET mechanisms - the neighboring- group mechanism neighboring -group participation by π and σ bonds - the SNi mechanism nucleophilic substitution at an allylic carbon - nucleophilic substitution at an aliphatic trigonal carbon - nucleophilic substitution at a vinylic carbon. Reactivitythe effect of substrate structure - the effect of the attacking nucleophile - the effect of the leaving group - the effect of the reacting medium - ambident nucleophiles ambident substrates.
- UNIT II: Aromatic nucleophilic substitution Reactions: SNAr mechanisms SN¹ mechanism-benzyne mechanism, SRN1 mechanism- other mechanism. Reactivity the effect of substrate structure, the effect of the leaving group and the effect of attacking nucleophile. Nitrogen nucleophiles amino dehalogenation Goldberg reaction.Halogen nucleophiles- halo-de-halogenation. Amino de hydroxylation Bucherer reaction- -Von Braun reaction—the Hurtley reaction Hydrogen as leaving group Zeigler alkylation Chichibabin reaction Schiemann reaction the Von-Richter rearrangement.
- **UNIT III: Oxidation and reduction:** Direct electron transfer, hydride transfer, hydrogen atom transfer, formation of ester intermediates, displacement mechanisms and addition-elimination mechanisms. Oppenauer oxidation, with *N*-Bromosuccinamide or related compounds- ozonolysis oxidative cleavage of double bonds and aromatic rings Lemieux-von Rudloff reagent- oxidation of aromatic side chains oxidative cleavage of alkyl groups from rings Dakin reaction- Baeyer-Villiger reaction oxidative decarboxylation bisdecarboxylation oxidation of methylene to carbonyl oxidation of arylmethanes. Catalytic reduction electrochemical reduction at low overvoltage at high overvoltage electrode photochemical reduction reduction by hydrazines homogeneous hydrogenation reduction by metal hydrides and alkoxides disproportionation reduction by dissolving metals
- UNIT IV: Stereo chemistry: Stereoisomerism.- Conformational analysis in acyclic and simple cyclic systems substituted ethanes, cyclohexane, cyclooctane and decalins, optical isomerism optical activity molecular dissymmetry Chirality of organic molecules with or without chiral centres. Specification of configuration in compounds having one or more stereogenetic centres. Enatiotopic and diastereotopic atoms, and faces. Stereoselective and stereospecific synthesis. Fischer's projection, D, L and R, S configurations relative and absolute configurations optical isomerism due to asymmetric carbon atoms optical isomerism in biphenyls, allenes and spirans, cycloalkenes optical isomerism of nitrogenous compounds racemisation and resolution geometrical isomerism and E, Z configurations, properties of geometrical isomers.
- **UNIT V:** Chemistry of Natural Products: Steroids structural elucidation and bio-synthesis of oesterone and progesterone. Vitamins -structural elucidation and bio synthesis of vitamin A and C.

References:

- 1. Advanced Organic Chemistry; Reactions, Mechanisms and Structure -Jerry March.
- 2. Reaction Mechanism in Organic Chemistry S. M. Mukherji and S. P. Singh.
- 3. Advanced Organic Chemistry; Part A Structure and Mechanisms Carey and Sundberg.

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SEMESTER – II

EC 1 - PHYSICAL CHEMISTRY I

Subject Code: 17P2C5EC	Credits: 5	External Marks: 75	Hours: 6
UNIT I: Introduction to Ou	antum Chemistry		

UNIT I: istry

Classical Quantum Theory - Quantum Theory of radiation-photoelectric effect- Bohr's Heisenberg Uncertainty principle- Compton Effect-Quantum quantum Theory mechanics-Postulates of quantum mechanics - functions -operators - Linear and Hermitian operators- eigen value- eigen function- solving eigen values by secular equations and similarity transformation methods - The Schrodinger wave equationapplication of Schrodinger wave equation - Particle in a box (one and three dimensional systems).

UNIT II: **Applications of Quantum Chemistry**

Concept of Orthogonalization and normalization- the origin of quantum numbers (angular momentum and spin) Applications of Schrodinger wave equation for multielectron atom -Variation and Perturbation methods- application of variation method to hydrogen molecule and application of perturbation method to helium atom. Molecular Quantum mechanics - Valence bond theory for hydrogen molecule - Molecular Orbital theory for di- and polyatomic molecules.Born - Oppenheimer approximation.

UNIT III: **Chemical Kinetics**

Theories of reaction rates: Simple Collision Theory, Absolute Reaction Rate Theory applications to bimolecular and termolecular reactions. Theory of unimolecular reactions - Lindeman's theory, Hinshelwood theory. Primary and secondary kinetic isotope effects - steady state approximation - chain reactions - thermal and photochemical reactions between hydrogen and halogens - H2-O2 reaction - Rice-Herzfeld mechanisms. Fast reactions- study of kinetics by stopped flow technique, relaxation method, flash photolysis and magnetic resonance method. Solution kinetics -Hammett and Taft equations.

UNIT IV: Surface Chemistry

Surface phenomena: Adsorption and free energy relationship at interfaces - heats of adsorption - Gibbs adsorption isotherm - physisorption and chemisorption - Freundlich, Langmuir and BET isotherms - Langmuir Hinshelwood mechanism - Langmuir Rideal mechanism. Study of surfaces - Surface area determination, surface films, adsorption from solution - study of kinetics of surface reactions - catalysis by metals, semiconductor, oxides - Gibb's adsorption equation - catalytic activity of surfaces-Adsorption of gases on solids.

Fundamentals of Catalysis UNIT V:

Concepts - classifications, mechanism and applications. Phase transfer catalysis - Super acid catalysis -sulphates, metal oxides. Enzyme catalysis - kinetics of enzyme catalysis, Neutral salt catalysis-primary salt effect - Bronsted-Bjerrum equation-secondary salt effect - Acid-base catalysis - catalysis by transition metal ions and their complexes supported transition metal complexes as catalysts - catalysis by enzymes - phase transfer catalysis - photocatalysis - adsorption - chemisorption on metals, metal oxides and semiconductors. Catalyst deactivation and regeneration.

References

- Introductory quantum chemistry, A.K.Chandra, Tata-McGraw Hill. 1.
- Quantum chemistry, R.K.Prasad, Wiley Eastern Ltd. 2.
- Molecular quantum mechanics, P.W.Atkins, Clarenden. 3.
- 4. Chemical applications of group theory, F.A.Cotton, Wiley eastern.
- Group theory and its applications in chemistry, K.V.Raman, Tata-McGraw Hill. 5.
- An Introduction to Electrochemistry by S. Glasstone. 6.
- Physical chemistry, P.W.Atkins, ELBS. 7.
- 8. Thermodynamics for students of chemistry, J.Rajaram & J.C.Kuriacose, Shobhen Lal Nagin Chand.
- 9. Thermodynamics for chemists, S.Glasstone, Affiliated East-West Press.
- 10. Chemical Kinetics, K.J.Laidler, Tata-McGraw Hill.

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SEMESTER – II

EC 2 - NANO MATERIALS & GREEN CHEMISTRY

Subject Code: 17P2C6EC	Credits: 4	External Marks: 75	Hours: 6
Objective			

To introduce the students about Nanochemistry and nanomaterials synthesis To teach the importance of characterization & applications of nanomaterials To teach the importance of green Chemistry

UNIT I: Chemistry of Materials

Synthesis of solid state materials using different techniques - ceramic techniques, coprecipitation techniques, sol gel techniques, precursor techniques, high temperature & high pressure synthesis. Purification and crystal growth: zone refining, growth from solution - preparation of semiconductors and applications. Oxide Films - Growth of oxide films, structure and physical properties; thin films-various stages of film growth, defects during growth, surface area and roughness; techniques of film growth.

UNIT II: Introduction to Nanotechnology

Basic nanotechnology science and chemistry concepts, nanoparticles- Size effects on Structure and Morphology; Synthesis of Nanomaterials and Nanoparticles - Top-down approach (physical vapor deposition, chemical vapor deposition) – bottom-up approach (sol-gel, co-precipitation, and hydrothermal methods) – growth mechanism (vapor- liquidsolid, solid-liquid-solid). Nanoporous Materials, nanocrystals, quantum dot, catalysts -Metal nanoparticles- Synthesis of Metal oxide nanoparticle; Study of nucleation and growth kinetics; Study on carbon-arch technique for production of carbon nanotube.

UNIT III: Properties & Applications of Nanotechnology

Physical and Chemical and Properties on the Nanoscale, some properties of nanomaterials like Magnetism, Electronic Structure in Clusters, Optical Properties, Mechanical, Super plasticity Chemistry; Techniques for Nanoparticle Characterization (TEM, SEM, and AFM). Application as sensors, biomedical applications, application in optics and electronics and electromagnetism - nanoparticles in polymers - Nanocatalysis (transition metal nanoparticles in catalysis, aerogel supported nanoparticle in catalysis, multi metallic nanoparticles in catalysis).

UNIT IV: Basic Principles of Green Chemistry

The need for green chemistry - Twelve principles of green chemistry, environmental protection laws, pollution control and pollution prevention – Prevention of waste by products, maximum incorporation of the reactants into the final product, prevention or minimization of hazardous products, recycling of waste. Solvent Free Organic Synthesis: Reactions on solid supports, phase transfer catalysis, reactions without support or catalyst. **Green Catalyst:** - Acid catalyst, oxidation catalyst, basic catalyst, polymer supported catalyst.

UNIT V: Green Synthesis & Applications

Designing Green Synthesis – choice of starting materials, choice of reagents, choice of catalysts – bio catalysts, polymer supported catalysts, choice of solvents. Synthesis involving basic principles of green chemistry – Examples – synthesis of adipic acid, synthesis of catechol, synthesis of methyl methacrylate, paracetamol. Microwave assisted reactions in water – oxidation of toluene to benzoic acid. Ultrasound assisted reactions – esterification, alkylation, oxidation, reduction reactions. Green chemistry in day to day life, industrial applications.

RECOMMENDED BOOKS

Solid State Chemistry by D. K. Chakrabarty.

1. Material Science and Engineering, V. Raghavan.

- 2.J. D. Lee, Concise Inorganic Chemistry, Elbs with Chapman and Hall, London
- 3.A.R. West, Plenum, Solid State Chemistry and its applications
- 4.R. Raghwan, First Course in Material Science
- 5.Kenneth. Klabunde, Nanoscale Materials in Chemistry, John Wiley & Sons, Inc. 2002
- 6.Rashmi Sanghi, M. M. Srivastava, Green Chemistry, Environment Friendly
 - Alternatives, Narosa Publishing House, 2007
- 7.V. Kumar, An Introduction to Green Chemistry, Vishal Publishing CO. Jalandhar, 2007

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SEMESTER – I

CC - PRACTICAL III INORGANIC CHEMISTRY II

Subject Code: 17P2CP3Credits: 4External Marks: 60Hours: 6

Gravimetric & Volumetric analysis

1. Estimation of Copper Volumetrically & Barium Gravimetrically

2. Estimation of Copper Volumetrically & Nickel Gravimetrically

3. Estimation of Calcium Volumetrically & Magnesium Gravimetrically

4. Estimation of Copper Volumetrically & Zinc Gravimetrically

Preparations

Preparation of simple complexes

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SEMESTER – II

CC - PRACTICAL IV PHYSICAL CHEMISTRY II

	Subject Code: 17P2CP4	Credits: 4	External Marks: 60	Hours: 6
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- 1. Determination of energy of activation for first order kinetics. (Hydrolysis of ester)
- 2. Relative strength of two acids from the study of hydrolysis of an ester.
- 3. Kinetics of the reaction between Potassium per sulphate Vs Potassium iodide (2nd order

kinetics)

- 4. Iodination of acetone (Zero order reaction)
- 5. Determination of molecular weight by Transition Temperature method.
- 6. Primary salt effect on 2nd order kinetics.
- 7. Adsorption isotherm
- 8. Phenol-Water system & effect on impurity the critical temperature

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SEMESTER – III

CC 5 - INORGANIC CHEMISTRY II

Subject	Code: 1	17P3	C7	C	redits	: 5	External Marks: 75	Hours: 6
					-	-		

UNIT I: Theories of Coordination Compounds

Crystal Field Theory (CFT) – splitting of d- orbitals under various geometries (octahedral, tetrahedral, tetragonal and square-planar) – factors affecting the splitting – crystal field stabilization energy calculation – Consequences of CFS – ionic radii of transition elements, heats of hydration, lattice energy- limitation – ACFT or LFT – Molecular Orbital Theory (MOT) - $\boldsymbol{\sigma}$ and $\pi \boldsymbol{\pi}$ bonding. John-Teller distortion

UNIT II: Stability and Electronic Spectra of Complexes

Stability of complexes: Stepwise stability constant and overall stability constant – factors affecting the stability of complexes –determination of stability constant by Job's variation method and polarographic method. Electronic spectra: Term symbols for d¹ to d⁹ ions – characteristics of d-d transition – energy level diagram – Orgal and Tanabe-Sugano diagrams – charge transfer spectra ORD – Cotton effect – Circular Dichroism – nephlauxetic effect – ESR and Maussbauer spectra.

UNIT III: Reactions of Complexes

Substitution reactions: Labile and inert complexes – ligand displacement reactions. $S_{\rm N}1,\ S_{\rm N}2$ & $S_{\rm N}1{\rm CB}$ mechanisms – substitution in square-planar complexes – Marcus Hush principle-trans effect – theories of trans effect - Electron transfer reactions: Inner sphere and outer sphere mechanisms – isomerization and recemization. Photochemical reactions of complexes – photosubstitution, photoreduction and photosensitization.

UNIT IV: Complexes of π Acceptor Ligand

Carbonyls (mono and polynuclear): EAN rule- Preparation and uses of metal carbonyl- nature of bonding in metal carbonyls. Nitrosyls – linear, bent and bridging – carbonyl nitrosyls – metal carbonyl halides (reparation and structure of Fe compounds). Organometallics and complexes of biological importance: 18 electron rule and Organometallic complexes- Olefinic and acetylinic complexes – arene complexes – catalysis by organometallics –Wilkinson's catalyst, Wacker process, oxo process, Ziegler-Natta catalyst, Fischer Tropsch's synthesis and Reppe's catalysis.

UNIT V: Crystal geometry and structure determination

Crystal geometry – Miller indices- Reciprocal lattice and its applications: structures of ZnS, Fluorite, Wurtzite, NiAs, CdI_2 , rutile, perovskite and spinel. Determination of crystal structure by powder X-ray diffraction and Rotating crystal method – interpretation and results. Neutron diffraction: An elementary treatment – application and comparison with X-ray diffraction. Electron diffraction: Basic principles and applications.

References:

Concept and models of Inorganic chemistry, B. E. Douglas, D.H. Mc Dani Waltham, Mass, 1965.

- 1. Introduction to Advanced Inorganic Chemistry, P.J. Durrant & B Durrant, Wiley.
- 2. Modern aspects of Inorganic Chemistry, 3/e, H.J. Emeleus, J.S.Anderson, Van Nostrand-Reinhold, New York, 1962.
- 3. Inorganic reactions and structure, E.S.Gould, Holt, Rinehart & Winston, New York, 1962.
- 4. Advanced Inorganic Chemistry: A comprehensive Text, 3/e, F.A. Cotton & G Wilkinson.
- 5. New concise Inorganic Chemistry, 2/e, J. D. Lee, Van Nostrand-Reinhold.
- 6. Inorganic Chemistry, K. F. Purcell & J. C. Kotz, Saunders, Philandelphia, 1977.
- 7. The Principles of inorganic Chemistry, W. L. Jolly, McGraw-Hill, New York, 1976.
- 8. Inorganic Chemistry: Principles of structure and reactivity, J.E. Huheey.
- 9. Basic Solid State Chemistry, A. R. West, John Wiley and Sons Ltd, 1999.

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SEMESTER - III

CC 6 - PHYSICAL CHEMISTRY II

Subjec	t Code: 17P3C8	Credits: 5	External Marks: 75	Hours: 6
Unit I:	Group Theory			

Principles of group theory: Symmetry elements, point groups, properties of a group, sub groups and classes – Abelian, cyclic and non-Abelian groups – symmetry operationsmultiplication tables, Classes of symmetry operations, basis, representative and matrix representations of operations. Molecular symmetry – similarity transformation -identification and determination; comparison of molecular and crystallographic symmetry; reducible and irreducible representations; direct product representation; orthogonality theorem- character table.

Unit II: Applications of group theory

Application of group theory in σ and π bond. Group theory orientations of ligand field theory – construction of energy level diagrams. Application of group theory in forming the selection rules for Infra-Red and Raman spectra- electronic spectra of ethylene and formaldehyde. Consequences of orthogonality theorem – construction of character table for C_{2V} and C_{3V} – hybrid orbitals in non linear molecules (CH₄, XeF₄, BF₃, SF₆ and NH₃). Determination of representations of vibrational modes in non linear molecules (H₂O, CH₄, BF₃, and NH₃).

Unit III: Electrochemistry I

Arrhenius theory of electrolytic dissociation, revision of basic electrochemistry (Types of electrodes and cells). Electrochemical cells with and without transference, determination of activity coefficients of an electrolyte, degree of dissociation, instability constant of silver ammonia complex. Mean ionic activity - ideal and non- ideal solutions; excess functions; Hydration number; Debye - Huckel theory of inter-ionic attraction , Debye-Huckel treatment of dilute electrolyte solutions; Debye-Huckel limiting law- Debye-Huckel-Onsager equation and its validity for dilute and concentrated solutions.

Unit IV: Electrochemistry II

Zeta potential - Polarization- types - over voltage - hydrogen and oxygen over voltage - Butler-Volmer equation - Tafel equation. Electrolysis - Decomposition potentials - calculations and determinations. Fuel cells – Batteries - primary and secondary fuel cells - significance of fuel cells- hydrogen - oxygen, hydrocarbon - air, natural gas and carbon monoxide, air fuel cells. Corrosion: concept and importance, mechanism of corrosion and Pourbaix diagrams - Evan's diagram – electrodeposition.

Unit V: Spectroscopy

Microwave spectroscopy and IR spectroscopy: The rotation of molecules - Stark effect – symmetric top molecules and asymmetric top molecules – isotopic effect – applications. The diatomic vibrating rotator interaction of rotations and vibrations – vibrations of polyatomic molecules isotopic substitution.

Raman spectroscopy: Raman effect – theory – pure rotational Raman spectra – vibrational Raman spectra – comparison of IR and Raman spectra – laser Raman spectroscopy – techniques and instrumentations (Principles only). Structural determinations of simple molecules.

Electronic spectroscopy: Vibrational Coarse structure – Frank-Condon principle – dissociation energy and dissociation products rotational fine structure of electronic vibrational transitions – The Fortrat diagram – pre-dissociation.

References

- 1. Chemical applications of group theory, F.A.Cotton, Wiley eastern.
- 2. Group theory and its applications in chemistry, K.V.Raman, Tata-McGraw Hill.
- 3. An Introduction to Electrochemistry by S. Glasstone.
- 4. Electrolytic Solutions by R. A. Robinson and R. H. Strokes.
- 5. Physical chemistry, P.W.Atkins, ELBS.
- 6. Chemical thermodynamics, T.M.Koltz, Benjamin.
- 7. Chemical Kinetics, K.J.Laidler, Tata-McGraw Hill.
- 8. Introduction to molecular spectroscopy, G.M.Barrow, McGraw Hill.
- 9. Molecular spectroscopy, C.N.Banwell, McGraw Hill.
- 10. Basic principles of spectroscopy, R.Chang, McGraw Hill.

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SEMESTER – III

EC 3 - ORGANIC CHEMISTRY - III

5	Subject Code: 17P3C9EC	Credits: 5	External Marks: 75	Hours: 6
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UNIT I: Molecular Rearrangements

Wagner Meerwin Rearrangement- Demyanovrearrangment - Hoffmann rearrangement - Curtius rearrangement - Losson- Schmidt reaction- Stevens – quinone-quinol rearrangement- Favorski rearrangement- Wallasch synthesis-Calisen rearrangement- Beckmaan rearrangement – Wolff rearrangement. Fries rearrangement - Baeyer Villiger rearrangement – Von-Richter rearrangement -Sommelet Hauser - Arndt-Eistert synthesis - Neber rearrangement Wittig reaction-Orton rearrangement - Sommelet - Hauser rearrangement-Bamberger rearrangement - the smiles rearrangement.

UNIT II: Organic photochemistry

Photochemistry of carbonyl compounds – Norrish type – I and II reactions (application oriented)- photo chemical reactions of cyclic ketones – Barton reaction, Paterno – Buchi reaction - photo chemistry of α , β nsaturated ketones-photo chemistry of olefins- cis – trans isomerisation – dimerization reaction – photo chemistry of butadiene- Zimmermann reaction- photo chemistry of α -santonin

UNIT III: Pericyclic reactions

Conservation of molecular orbital theory – symmetry properties of molecular orbital's – electrocyclic reactions – correlation diagram and FMO method – cyclo addition reactions – correlation diagram and FMO method- sigmatropic rearrangements- FMO method – applications of PMO methods to pericyclic reactions.

UNIT IV: Organic synthesis

Synthesis, reactions, mechanisms and selectivity involving the following – alkenes, alkynes, arenes, alcohols, phenols, aldehydes, ketones, carboxylic acids and their derivatives, halides, nitro compounds and amines- use of compounds of Mg, Li, Cu B and Si in organic synthesis- concepts in multistep synthesis – retro synthetic analysis - disconnections ethyl-indole-3-butyrate, ethylcinnamate – furo-maleate adduct. Synthetic equivalent, synthons - unpoloung – selectivity – protection and deprotection of functional groups

UNIT V: Biopolymers

Structure and functions of biopolymer such as proteins - primary, secondary and tertiary structures of proteins – enzymes classification - mechanism of enzyme action – structure of DNA and RNA.

References:

Advanced Organic Chemistry; Reactions, Mechanisms and Structure -Jerry March.

- 1. Reaction Mechanism in Organic Chemistry S. M. Mukherji and S. P. Singh.
- 2. Advanced Organic Chemistry; Part A Structure and Mechanisms, -Carey and Sundberg.
- 3. Organic Reactions and their mechanisms P. S. Kalsi.
- 4. A guide book to mechanism in organic chemistry Peter Sykes.
- 5. Organic Chemistry, Volume I- I. L. Finar.
- 6. Organic Chemistry, Volume II- I. L. Finar.

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SEMESTER – III

EC 4 - SCIENTIFIC RESEARCH & ANALYTICAL TECHNIQUES

Subject Code: 17P3C10EC	Credits: 4	External Marks: 75	Hours: 6
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Objectives:

To provide completing the Master of Chemistry will be acquired knowledge, general competence and analytical skills at an advanced level targeting future employment in research, industry, teaching or public administration.

UNIT-I: Introduction of Research

Nature and importance of research - aims, objective, motivations in research, significance of research, research methods v/s methodology, criteria of good research, selection of research problem, Sources - primary and secondary sources - Survey of scientific literature – primary and secondary sources – current literature methods – identification and selection of research problems – experimental design – writing scientific papers -citation index for scientific papers and journals – writing of thesis - preparation of tables and figures – referencing.

UNIT-II: Research Specialization

Physical properties useful in analysis and methods of separation prior to analysis - Isolation techniques - extraction - Soxhlet extraction, crystallization, sublimation - methods for vacuum sublimation and distillation under reduced pressure. Separation of non-metals and metals - Ion Exchange separation: Theories of ion exchange, separation of halides and Rare earths.

UNIT-III: Evaluation of Analytical Data

Definition of Terms – Mean Median, Precision, accuracy - Reliability - Errors in chemical analysis, determinate and random errors - distribution of random errors - Average deviation and standard deviation, variance and confidence limit- Least square method. Methods of sampling: samples size - Techniques of sampling of gases, fluid, solids, and particulates.Statistical treatment of finite samples - the students test and F test - Criteria for rejection of an observation - the Q test, significant figures and computation rules - data plotting - least square analysis.

UNIT-IV: Chromatographic & Thermal Method Of Analysis

General principle, classification of chromatographic methods - Thin layer chromatography: coating of materials, preparative TLC. Solvents used and methods of detection Column chromatography: Nature of column materials -Preparation of the column. Column efficiency and resolution - Solvent systems and detection methods Thermogravimetry [TG], differential thermal analysis [DTA], differential Scanning calorimetric [DCS] - applications of thermometric titrations.

UNIT-V: Nephelometry & Turbidimetry:

Theory, Instrumentation – determination of sulphate and phosphate - Application in organic, inorganic, biological fluids and pollution analysis - Turbidimetric titrations – determination of molecular mass of high polymers.

Flurometry: Theory, Instrumentation – relation between intensity and concentration. Measurement of fluorescence – filter fluorometer – spectrofluorometer – advantages, limitations – reporting fluorescence spectra – application of fluorometric analysis – organic, inorganic and biological

RECOMMENDED BOOKS

Research Methodology. Methods and Techniques: C. R. Kothari.

- 1. Tests, Measurements and Research Methods in Behavioral Sciences: A. K.Singh.
- 2. Thesis and Assignment writing by Anderson.
- 3. K.Eckschlager, "Errors measurement and results in chemical Analysis" Reinhold Company.
- 4. A.I Vogel, Text Book of Quantitative Inorganic Analysis, Pearson V Edn., 2001.
- 5. Instrumental methods of chemical analysis by Chatwal. K, Anand, 5th edition.
- 6. Instrumental Methods of Chemical Analysis B. K. Sharma 9th Edition.

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SEMESTER – III

CC - PRACTICAL V ORGANIC CHEMISTRY I

Subject Code: 17P3CP5	Credits: 4	External Marks: 60	Hours: 6	

Separation and Analysis of organic mixture of two substances

Single stage preparation of organic compounds with green chemistry approach – purification and recrystallization

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SEMESTER – IV

CC 7 - PHYSICAL CHEMISTRY III

Subject Code: 17P4C11 Credits: 5 External Marks: 75 Hours: 6
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Unit I: Thermodynamics

Second law of thermodynamics; Physical significance of entropy, efficiency of heat engine, coefficient of performance of heat engine. Gibbs-Helmholtz equation; Third law of thermodynamics. Gibbs-Duhem equation, Maxwell relations, thermodynamic equation of state, chemical potential, variation of chemical potential with temperature & pressure-applications of chemical potential. Thermodynamics of ideal and real gases- thermodynamics of ideal and non ideal solutions - Rault's law, Duhem-Margules equation and its applications.

Unit II: Statistical Thermodynamics

Introduction- Maxwell - Boltzmann distribution law, Bose-Einstein and Fermi-Dirac statistics. Partition function – molecular – translational – rotational – vibrational and electronic partition function - thermodynamic functions in terms of partition functions-application of partition function to heat capacity of ideal gases.Heat capacity of solids – Einstein theory and Debye theory – Debye T – Cubed law.

Unit III: Crystalline and Amorphous Polymers

Crystalline and amorphous polymers-factors affecting crystallinity - effect on polymer properties. Glass transition temperature- thermal transitions-Determination of Tg and Tm – factors affecting Tg Polymer characterization by IR, NMR, TGA, DTA and DSC – Molecular weight of polymers and its distribution – molecular weight determination by GPC and Viscosity measurement- Mark – Houwink equation.

Unit IV: Specialty Polymers

Interpenetrating polymer net works (IPN) - Heat resistant polymers – Ladder polymers conducting polymers – photocrosslinking polymers - liquid crystalline polymers - Bio-compatible polymers – polymer composites - polymers for optical storage devices. Processing of Polymers- Compounding of polymers, moulding techniques – compression, injection, extrusion, blow moulding, rotational moulding, thermoforming, vacuum forming, calendaring, casting, reaction injection moulding, injection blow moulding and lamination.

UNIT V: Photochemistry

Photophysical process in electronically excited molecules – Jablonski diagram – Stern – Volmer equation and its applications – Experimental techniques – Chemical actinometers – Laser and its applications. Fluorescence mechanism – resonance fluorescence – sensitized fluorescence – Quenching of fluorescence – applications. Phosphorescence – mechanism. Photosensitization- Photosynthesis. Photocatalysis – principle – applications

References

- 1. Thermodynamics for chemists, S.Glasstone, Affiliated East-West Press.
- 2. Statistical Thermodynamics, Lee Sears & Turcotte, Addison Wesley.
- 3. Physical chemistry, P.W.Atkins, ELBS.
- 4. Chemical thermodynamics, T.M.Koltz, Benjamin.
- 5. V.R.Gowariker, N.V.Viswanathan and JayadevSreedhar, "Polymer Science" New Age
- 6. International (p) Ltd., New Delhi (2010).
- 7. F.W.Bill Mayer, "Text Book of polymer science" 3rd Edition John Wiley & sons, Inc., New York (2011).
- 8. Rohatgi Mukherjee, Fundamentals of Photochemistry, 2nd edition, New Age International (2004).

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SEMESTER – IV

CC 8 - APPLICATIONS OF SPECTROSCOPY AND CHEMISTRY OF SECONDARY METABOLITES

- Subject Code: 17P4C12 Credits: 5 **External Marks: 75** Hours: 6 Applications of UV-Visible and IR Spectroscopy in Organic Chemistry: UV-UNIT I: Visible spectroscopy: Various electronic transitions (185-800nm) - Ultraviolet bands for carbonyls compound - unsaturated carbonyl compounds, dienes, conjugated polyenes. Fischer-Woodward rules for conjugated dienes and carbonyls compounds - ultraviolet spectra of aromatic and heterocyclic compounds.IR Spectroscopy: Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, esters, phenol and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds).Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance.
 - UNIT II: Applications of NMR Spectroscopy in Organic Chemistry: PMR spectroscopy: General introduction and definition – chemical shift – spin-spin interaction – shielding mechanism – chemical shift values and correlation of protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides and mercapto) – Simplification of complex spectra – nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier Transform technique, Nuclear Overhauser Effect (NOE), C13 NMR chemical shift (aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbon)Coupling constant- application to structural elucidation of simple organic compounds.
 - UNIT III: Applications of Mass Spectroscopy in Organic Chemistry: Application of Mass Spectroscopy: FD and FAB factors affecting fragmentation – ion analysis – ion abundance. Mass spectral fragmentation of organic compounds – common functional groups – molecular ion peak – metastable peak – McLafferty rearrangement. Nitrogen Rule – high resolution mass spectroscopy. Examples of mass spectral fragmentation of organic compounds with respect to their structural determination.
 - UNIT IV: Synthesis and structural elucidation of natural phenolic and additive aromas: Secondary metabolites -Isolation, synthesis and reactivity of flavones, iso-flavones, chromones, coumarins and anthocyanins – basic fraction. Terpenoids - structural elucidation, disconnection approach and synthesis of Zingiberene, squalene, limonene and camphor.
 - **UNIT V: Synthesis and structural elucidation of some common alkaloids:** Tests for alkaloids –Isolation of alkaloids- Acid fraction- qualitative analysis of alkaloids with respect to functional groups stereochemistry of nitrogen compounds Zeisel method Herzig-meyer method- Hoffmann's exhaustive methylation Emde degradation- Von Braun's method- structural elucidation, disconnection approach and synthesis of nicotine, perlolidine and acronycine Synthesis of cryptosanguinolentine through Fischer-indole method.

References:

- 1. Introduction to Spectroscopy D.L. Pavia, G. M. Lampman, G. S. Kriz and J.A. Vyvyan.
- 2. Organic Chemistry Vol I & II, I.L.Finar.
- 3. Organic Spectroscopy R. M. Silverstein.
- 4. Chemistry of Natural Products Vol I & II, O.P.Agarwal.
- 5. Organic Chemistry of Natural Products Vol I & II, G.R. Chatwal.
- 6. Ph.D. Thesis Dr.P.Pitchai Submitted to Bharathiar University, Coimbatore (April 2009).
- 7. Ph.D. Thesis -Mr. A. Nepolraj-Submitted to Bharathidasan University Trichy(Dec-2016).
- 8. Ph.D. Thesis Mr. M. Sathiyaseelan Submitted to Bharathidasan University Trichy (Dec-2016).

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SEMESTER – IV

EC 5 - FOOD & MEDICINAL CHEMISTRY

- Subject Code: 17P4C13ECCredits: 4External Marks: 75Hours: 6UNIT I:Food and Nutrients: Foods classification proximate principles invalid foods –
nutritive properties of vegetables –nutrition properties of meat, fish and oil of sea
foods. Carbohydrates: Classification –carbohydrates in diets digestion and
absorption regulation of blood glucose insulin adrenaline. Protein: Sources
and chemical nature amino acids nitrogen balance factors affecting nitrogen
balance physiological needs dietary sources biological tests requirements –
protein deficiency. Fats: Visible & Invisible fats phospholipids digestion and
absorption essential fatty acids (EFA) deficiency dietary needs for fat.
 - UNIT II: Electrolytes, Minerals and Vitamins :Salt: Na and K in the body. Water balance

 Na excess K deficiency K excess. Minerals intake absorption substances
 recommended intake trace elements iodine physiology sources therapeutic uses fluorine prevention of dental caries, fluorosis in man fluoride
 and osteoporosis opposition to fluoridation of water Pb Hg Hazards.
 Vitamins: Vitamins classification source, physiological functions of vitamin A,
 D, E, K, B-complexes (B₁, B₂, B₆ and B₁₂), folic acid and vitamin-C.
 - **UNIT III: Drug design:**History of organic medicinal compounds, various routes of administration definition of allergy, side effects. Factors influencing drug metabolism and metabolic changes in drugs. Drug interactions non specific and specific interactions. Relationship of chemistry and biological activity. Development of new drugs, procedures followed in drug design, concepts of prodrugs and soft drugs. Theories of drug activity, Quantitative structure activity relationship. Concepts of drug receptors.
 - UNIT IV: Analgesics: Classification -narcotic analgesics Opium derivatives -Uses and toxic effects of morphine and codeine antipyretic analgesics paracetamol, phenacetin uses. Salicylic acid derivatives aspirin uses and toxic effects. Anti inflammatory- ibuprofen and indo methacin -uses and toxic effects. Synthetic drugs pethidine and methadones uses and side effects. Antibiotics: Introduction classification Penicillin, streptomycin and chloramphenicol structure and uses.

Anti malarial: Quinine, Trimethoprim- structure, uses and toxic effects.

UNIT V: A general study of the following classes of compounds: Histamines and anti histamines, Sedatives, hypnotics and tranquilizers, Antiseptics and disinfectants, Anti radiation and anti cancer drugs- Recent development in cancer chemotherapy- Hormones and natural products. Antitubercular & antileprotic -Ethambutol, Isoniazide & Dapsone. Cardiovascular - Synthesis of dilliazem, quinidine, methyldopa, atenolol, oxyprenol. AIDS: General study – symptoms – prevention & treatment.

References

- 1. Fundamentals of Nutrition, Corinne H. Robinson, Macmillan Publishing Co., Inc.
- 2. Food Science and Experimental Foods, M.Swaminathan, Ganesh & Co.
- 3. Food and Nutrition Vols 1&2, M.Swaminathan, BAPCO.
- 4. Goodman and Gillman, Pharmacology and Pharmacothearputics.
- 5. Ashutosh Kar, Medicinal Chemistry, Wiley Eastern, Madras.
- 6. Harkishan Singh and V.K.Kapoor, Organic Pharmaceutical Chemistry, Vallabh Prakashan, Delhi.
- 7. I.L.Finar, Organic Chemistry Vol. II, ELBS.
- 8. Bentley and Driver, Text book of pharmaceutical chemistry, 3rd edn,
- 9. Jayashree Ghosh, A Textbook of Pharmaceutical Chemistry, 1st edn.

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SEMESTER – IV

CC - PRACTICAL V ORGANIC CHEMISTRY II

Subject Code: 17P4CP6	Credits: 4	External Marks: 60	Hours: 6

a) Organic Estimation

- 1. Estimation of phenols
- 2. Estimation of anilines
- 3. Estimation of ketones
- 4. Estimation of Glucose
- 5. Estimation of Ascorbic acid

b) Double stage preparation of organic compounds

- 1. Hoffmann rearrangement of aromatic amides with household bleach and acetylation of the resultant amines with acetic anhydride.
- 2. Hoffmann rearrangement of aromatic amides with household bleach and bromination of the resultant amines.
- 3. N-Bromination of acetanilide with $Br_2/NaOH$ mixture; and the Orton rearrangement of respective N-bromoacetanilide.
- 4. N-Acetylation of aromatic amines and bromination of the resultant product.

Comparative thin layer chromatographic slides must be shown for the products of 3^{rd} and 4^{th} experiment. (**Only for Class Observation**)

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SEMESTER – IV

PW – PROJECT WORK

Subject Code: 17P4CPW	Credits: 5	External Marks: 80	Hours: 6