DEPARTMENT OF CHEMISTRY

CHOICE BASED CREDIT SYSTEM (CBCS)

OUTCOME BASED EDUCATION SYLLABUS

M.Sc. CHEMISTRY

2020 - 2021 BATCH

DWARAKA DOSS GOVERDHAN DOSS VAISHNAV COLLEGE
(AUTONOMOUS)
College with Potential for Excellence
Linguistic Minority Institution Affiliated to University of Madras
E.V.R. PERIYAR HIGH ROAD,

ARUMBAKKAM, CHENNAI – 600106, TAMILNADU.

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D.G.VAISHNAV COLLEGE

VISION

To impart value-based quality academia; to empower students with wisdom and to charge them with rich Indian traditions and culture; to invoke the self, to broaden the same towards nation building, harmony and universal brotherhood

MISSION

To ensure sustained progress and development in imparting quality education, to pioneer new avenues of teaching and research and to emerge as an institution with potential for excellence

DEPARTMENT OF THE CHEMISTRY

VISION

To impart a sound **knowledge** in chemistry to the students that stresses scientific reasoning and problem-solving skills. To equip students with the **skills** required to strengthen their social responsibility and to make them competent in this knowledge-driven society.

MISSION

M1	To educate students with state-of-the-art curriculum, improvised teaching methodologies and progressive research facilities. To expose students to a breadth of experimental techniques this will transform them into quality chemist.
M2	To produce socially responsible chemist who can contribute more to the industry and to address problems of societal importance. To make the department a thriving center of excellence in teaching, curriculum development and valuable research
M3	To outreach the under-privileged students of the city in the form of workshops, on-line courses, etc that showcase the role of chemistry as central science.

Eligibility for admission to M.Sc.

Pass in B.Sc. Chemistry examination, degree awarded by recognized Indian Universities with Mathematics and Physics, as the allied subjects.

Duration of course

M.Sc. (Two years)

Eligibility for the award of degree

Eligibility for the award of degree: Passing of all the subjects (both in internal and ESE) offered by the college for the course.

PROGRAM EDUCATION OBJECTIVES (PEOs)

PEO1	To produce efficient and intellectual undergraduates with strong fundamentals in organic, inorganic, physical and analytical chemistry to pursue higher studies in the field of research, innovation and technology
PEO2	To make undergraduates, capable of attaining employment in teaching and industry.
PEO3	To enable postgraduates to develop professionally through life-long learning, higher education and other creative entrepreneurial pursuits in their areas of expertise or interest**.**
PEO4	
PEO5	

PEO TO MISSION STATEMENT MAPPING

MISSION STATEMENTS	PEO1	PEO2	PEO3	PEO4	PEO5
M1	3	2	3		
M2	2	1	3		
M3	2	2	3		

CORRELATION: 3- STRONG 2- MEDIUM 1- LOW

PROGRAMME OUTCOMES

At the completion of the M.Sc. Chemistry program, the students of our Department will be able to :

S.NO	GRADUATE ATTRIBUTES	PROGRAMME OUTCOMES
1.	**Knowledge**	Attain in depth knowledge about the fundamental principles, essential facts, conclusions and applications of chemical and scientific theories in various domains of chemistry. **(PO1)**
2.	**Critical Thinking**	Carry out experiments in the area of organic analysis, estimation, derivative process, inorganic semi micro analysis, preparation, Kinetic, conductometric and potentiometric experiments and spectral analysis applying the domain of critical thinking. **(PO2)**
3.	**Problem Solving**	Define the background of reaction mechanisms, complex chemical structures, instrumental method of chemical analysis, and separation techniques and apply appropriate techniques for analysing specific problems both qualitatively and quantitatively in laboratories and in industries. **(PO3)**
4.	**Usage of modern tools**	Create data using modern chemical tools and ICT for modeling and analyze the data obtained from sophisticated instruments (like UV-Vis , FTIR, NMR, GCMS, Fluorescence, SEM,TEM and XRD) for chemical analysis **(PO4)**
5.	**Communication**	Develop Skills to evaluate, analyze and interpret the chemical information and data and to communicate effectively within the chemical community and with society at large, such as, being able to comprehend and write effective reports and design documentation, make effective presentations, and give and receive clear instructions. **(PO5)**
6.	**Life-long Learning**	Demonstrate scholarly attitude to pursue a career in the field of chemical education and research and have the zeal and vision to engage in independent and life-long learning in the broadest context of technological and social change. **(PO6)**
7.	**Ethical Practices and Social Responsibility**	Generate ideas and solutions for green and sustainable chemistry and approach towards planning and execution of research in frontier areas of chemical sciences. **(PO7)**
8.	**Independent and Reflective Learning**	Develop entrepreneurial skills in interdisciplinary and multidisciplinary areas of chemical sciences and its applications and develop a zeal to pursue a career in the field of chemistry.**(PO8)**

Mapping of POs TO PEOs

PEO/PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7
PEO 1	3	2	2	2	2	2	1
PEO 2	2	2	3	1	2	2	3
PEO 3	2	3	3	2	1	1	3
PEO 4	3	2	2	2	1	1	2
PEO 5	2	2	2	3	2	2	1

3-Strong Correlation 2- Medium Correlation 1- Low Correlation

PROGRAM SPECIFIC OUTCOMES (PSO's)

At the time of graduation, our post graduates would be able to:

PSO1. Create, Evaluate, analyze, interpret and effectively apply the basic laws, principles, phenomena, processes and mechanisms involved in the domain of Chemistry

PSO2. Apply the knowledge of chemistry in the domain of advanced research, education and perspective entrepreneurship.

PSO3. Solve the complex problems in the field of chemical data analysis, scientific interpretation reaction mechanisms with an understanding on tools to be employed and analytical skills to be applied with proper insight on societal, environmental, safety, legal and cultural impacts of the solution.

PSO4. Apply the knowledge of chemistry to appreciate, develop and test the theoretical aspects for applications in energy, environment, materials, medicines, and technology.

PSO5. Use standard laboratory equipments, modern instrumentation and classical techniques to carry out experiments and develop skills to interpret and explain the validity of experimental data in terms of accuracy and underlying theory.

SYLLABUS & SCHEME OF EXAMINATION - M.Sc. CHEMISTRY 2020– 2021 BATCH

SEM	PART	TITLE OF THE PAPER	INSTRUCTION HOURS/WEEK	DURATION OF EXAM	MAX. MARKS			CREDITS
					CIA	ESE	TOTAL	
SEMESTER-I								
I	Core I	Organic Chemistry – I	6	3	40	60	100	4
	Core II	Inorganic Chemistry-I	6	3	40	60	100	4
	Core III	Physical Chemistry-I	6	3	40	60	100	4
	Soft Skill I	-	-	3	40	60	100	2
SEMESTER-II								
II	Core IV	Organic Chemistry-II	6	3	40	60	100	4
	Core V	Inorganic Chemistry-II	6	3	40	60	100	4
	Core VI	Physical Chemistry-II	6	3	40	60	100	4
	Core VII	Organic Chemistry Practical - I*	7	6	40	60	100	4
	Core VIII	Inorganic Chemistry Practical – I*	7	6	40	60	100	4
	Elective I	Physical Chemistry Practical – I* OR Computational Chemistry	5	6	40	60	100	3
	Soft Skill II	-	-	3	40	60	100	2
	Advanced Course	Analytical Chemistry Practical-I*	5	6	40	60	100	3
	Open Elective	Seminar	7	-	-	-	-	3
SEMESTER-III								
III	Core IX	Organic Chemistry-III	6	3	40	60	100	4
	Core X	Inorganic Chemistry-III	6	3	40	60	100	4
	Core XI	Physical Chemistry-III	6	3	40	60	100	4
	Soft Skill III	-	--	3	40	60	100	2
		Internship (not less than 4 weeks)	-	-	-	-	-	2
SEMESTER-IV								
IV	Core XII	Organic Chemistry-IV	6	3	40	60	100	4
	Core XIII	Inorganic Chemistry-IV	6	3	40	60	100	4
	Core XIV	Physical Chemistry-IV	6	3	40	60	100	4

	Core XV	Physical Chemistry Practical II*	5	6	40	60	100	4
	Elective II	Organic Chemistry Practical II* **OR** Research Methodology	7	6	40	60	100	3
	Elective III	Inorganic Chemistry Practical II* **OR** Modern Instrumental Techniques	5	6	40	60	100	3
	Soft Skill IV	-		3	40	60	100	2
	Advanced Course	Analytical Chemistry Practical-II*	5	6	40	60	100	3
		Group Project / Review*	-	6	40	60	100	3
	TOTAL CREDITS Elective:12 CORE: 60 Soft skill: 8 Advanced course:6 Group project:3 Seminar: 3 Internship: 02							**94**

COURSE TITLE: CORE I – ORGANIC CHEMISTRY – I

Course Code	**: 1923101**	**Credits**	**: 04**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

This course aims to explain basic concepts in stereo chemistry and conformational analysis of organic molecules. In addition, the reaction mechanism and synthetic application of aliphatic and aromatic substitution reactions in organic synthesis will be discussed in detail.

COURSE OUTCOMES:

At the end of the Course, the Student will be able to:

CO1	Visualize and draw the design of atoms in space in 3D orientation.
CO2	Compare the importance of pharmacokinetic profiles of enantiomers especially used in chiral pharmaceuticals.
CO3	Apply conformational analysis for predicting physico-chemical properties and molecular modeling in screening compounds for biological activity.
CO4	Interpret the concept of aromatic electrophilic and nucleophilic substitution and its effective usage in organic synthesis.
CO5	Recall the organic effects like inductive, resonance and steric effects and its influence in reaction rates and derive the Hammett and Taft equations.
CO6	Assess the reaction mechanism involved using Hammett and Taft and helps to derive quantitative structural relationships for organic compounds.

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	PO										PSO				
	1	2	3	4	5	6	7	8	9	10	1	2	3	4	5
CO1	3	3	3	3	3	3	3	3	3	3	3	3	3	3	2
CO2	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
CO3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
CO4	3	3	3	3	3	2	3	3	3	3	3	3	3	3	2
CO5	3	3	3	3	2	2	3	3	3	3	3	3	3	2	2
CO6	3	3	3	3	2	2	3	3	3	3	3	3	3	2	2

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	CONTENTS OF MODULE	Hrs	COs
1	**STEREOCHEMISTRY** 1.1 Stereoisomerism and stereo isomers -Terminology - symmetric, asymmetry, dissymmetry, Prochiral, Chiral, achiral. Chirality and Stereogenic centres, Optical activity – interaction of plane polarized light with optical isomers. 1.2 Topicity and Prostereoisomerism – Identification of homotopic, enantiotopic, diastereotopic atoms /groups, Re and Si faces in simple molecules. 1.3 Axial, planar and helical chirality- A study of dissymmetry of allenes, biphenyls, spiro compounds, trans cyclooctene, cyclononene, Binaphthyls, Cyclophanes, ansa-compounds, and molecules with helical structures. 1.4 Configurational nomenclature (R/S) of simple carbocyclic compounds, Biphenyls, allenes, spiranes, alkylidene cycloalkanes and helicenes.	**18**	**CO1, CO2**

	1.5 Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst-controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution by optical method. Crams rule, optical purity. Stereoselectivity, stereospecificity, Enantioselectivity, diastereoselectivity, Regioselectivity and regiospecificity. 1.6 Geometrical isomerism- E-Z nomenclature of higher order (substituted and branched) olefins. Geometrical and optical isomerism of disubstituted cyclopropane, cyclobutane and cyclopentanes.		
2	**CONFORMATIONAL ANALYSIS** 2.1 Conformation and stability – 1, 2-disubstituted ethane derivatives. Conformational analysis of di-substituted cyclohexanes and their stereo chemical features [geometric and optical isomerism (if shown) by these derivatives]. 2.2 Conformation and reactivity a. Iodide induced di-debromination of dl/threo- and meso-2,3-dibromobutanes b. Dehydrobromination of threo- and erythro-1-Bromo-1,2-diphenylpropane c. Reaction of 3-Bromo-2-butanols with HBr d. Reaction of 2-Aminocyclohexanols with HNO_2 e. Substituted cyclohexanols (oxidation and acylation) f. Cyclohexane carboxylic acids (esterification and hydrolysis) 2.3 Conformation and stability-2-halocyclohexanones and Alkyl substituted cyclohexanones. – Solvent effects. 2.4 Conformation and stereochemistry of cis and trans decalin, 9-methyl decalin 2.5 Chemical consequence of conformational equilibrium – Curtin - Hammet principle	**18**	**CO3**
3	**ALIPHATIC NUCLEOPHILIC SUBSTITUTION REACTIONS** 3.1 Reactive intermediates: Carbocations, carbanions, free radicals carbenes, nitrenes, and arynes, - Generation, detection, stability and reactivity.	**18**	**CO4**

	3.2 SN_1, SN_2 and SN_i, SN_1', SN_2' and tetrahedral mechanisms- reactivity, structural and Solvent effects, Neighboring group participation 3.3 Substitution in norbornyl and bridgehead systems – Bredts rule- substitution at allylic and vinylic carbons 3.4 Substitution at carbon doubly bonded to oxygen and nitrogen - Regioselectivity - ambident nucleophiles such as CN, NO_2, phenoxide and ambident dianions 3.5 Alkylation and acylation of amines, halogen exchange, Von-Braun reaction 3.6 Alkylation and acylation of active methylene carbon compounds, hydrolysis of esters, Claisen and Dieckmann condensations.		
4	**AROMATIC ELECTROPHILIC SUBSTITUTION REACTIONS** 4.1 The arenium ion mechanism – evidences. Orientation and reactivity (ortho, meta and para directing groups). kinetic isotope effects, structural effects on rates, the ortho- para selectivity ratio 4.2 Typical reactions mechanism to be studied with energy considerations - nitration, sulphonation, halogenation, alkylation, acylation and diazonium coupling. Electrophilic substitution via enolization, Stork-enamine reaction. Relationship between kinetic and thermodynamic stability – Hammond postulate 4.3 Formylation reactions - Gatterman, Gatterman-Koch, Vilsmeyer-Hack & Reimer-Tiemann Reaction,Jacobson reaction. 4.4 Synthesis of di & tri substituted – 1,2,3 tribromobenzene,2-methyl benzoic acid, 4-amino-2- hydroxybenzoic acid,p-formyl benzaldehyde,o-hydroxy anisole ,2-(4-isobutyl phenyl) propanoic acid (brufen). 4.5 Electrophilic substitution - Indole, quinoline, isoquinoline – orientation, reactivity – Comparative study of aromaticity and reactivity with pyrrole and pyridine.	**18**	**CO4**
5	**AROMATIC NUCLEOPHILIC SUBSTITUTION REACTIONS AND DETERMINATION OF REACTION MECHANISM** 5.1 Aromatic Nucleophilic Substitution - Methods for the generation of benzyne intermediate and reactions of aryne intermediate. Unimolecular and bimolecular mechanism-benzyne mechanism – Von Ritcher reaction, Vicarious Nucleophilic Substitution (VNS).	**18**	**CO2, CO5 and CO6**

	5.2 Nucleophilic substitution involving diazonium ions. Aromatic Nucleophilic substitution of activated halides. Ziegler alkylation. Chichibabin reaction – reactions of 2, 4 DNB, FDNB. 5.3 Kinetic and Non-Kinetic methods of determining organic reactions mechanisms. Non-kinetic methods. Energy profile diagrams, intermediate versus transition state, identification of products, Cross-over experiments, Stereo chemical studies - uses of isotopes. Kinetic methods: kinetic isotopic effects, salt effects, solvent effects- solvent isotopic effects, kinetic and thermodynamic controlled products, Curtin-Hammett principle. 5.4 Linear free energy relationship - Hammett equation, Significance of substituent constant (sigma) and reaction constant (rho) for substituted benzoic acid. Taft equation, acidity of carboxylic acids and phenols, basicity of aliphatic and aromatic bases.		

REFERENCES & TEXT BOOKS

1. Eliel E., Wilen S.H. and Mander L.N., Stereochemistry of Carbon Compounds, 2nd Edition, John Wiley & Sons, New York, 1994.
2. Nasipuri, Stereochemistry of Organic Compounds – principles and applications, 3rd Edition, New age Publications Ltd., New Delhi, 2011.
3. Kalsi P.S., Stereochemistry Conformation and Mechanism, 6th Edition, New age Publications Ltd., New Delhi, 2005.
4. Kalsi. P.S., Stereochemistry and Mechanism through Solved Problems, 4th edition, New age Publications Ltd., New Delhi, 2006.
5. Nimai Tewari, Advanced organic chemistry (problems and solutions), Books and Allied (P) Ltd., 2010.
6. Bruckner. R., Advanced Organic Chemistry, Reaction Mechanism, Elsevier, New Delhi, 2002
7. Carey F. A., Sundberg R. J., Advanced Organic Chemistry, Part A and Part-B, 5th Edition, Plenum Press, New York, 2007.
8. March J. Advanced Organic Chemistry, 4th Edition, John Wiley & Sons, Singapore, 1992.
9. Gilchrist T.L. and Rees C.W., Carbenes, Nitrenes and Arynes, Thomas Nelson and Sons Ltd., London, 1969.
10. Gilchrist T. L. Heterocyclic Chemistry, 2nd Edition, Longman, Essex, England, 1992.

11. Joule J.A. and Mills K., Heterocyclic Chemistry, 4th Edn, Backwell Science Publishers, England, 2000.
12. Rajbir singh, Physical organic chemistry, Mittal publications, 2002.
13. Anslyn, E.V, Dougherty D.A., Modern physical organic chemistry, University science books, 2006.
14. Jonathan Clayden, Nick Greeves & Stuart Warren, Organic Chemistry, Second Edition, Oxford University press.

WEBSITES:

1. http :// info dome . sdsu, ./research/ guides/ science/ org chemistryblr. html
2. http :// www.liv.ac.uk/chemistry/links /reactions.html
3. http ://orgchem.chem..uconn.edu/namereact/named.html
4. www.gcocities.com/ chempen softwar4ee/reactions.html

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**CIA I**	**CIA II**	**CIA III**	**ESE**
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

COURSE TITLE: CORE II – INORGANIC CHEMISTRY – I

Course Code	**: 1923102**	**Credits**	**: 04**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVE:

This course provides an ideal platform to explain the basic concepts on the structure, shape, bonding characteristics of simple inorganic compounds essentially comprising from p and d block elements that form clusters, rings, sheets, frameworks and cages. In addition to the structural aspects a basic introduction about the various theories pertaining to coordination complexes are dealt in detail focusing on the stereo and structural isomerism concepts in six and four coordinate metal complexes. Further, a wide application of the concept of bonding in organometallic chemistry and the application of these inorganic complexes as catalyst will be discussed in detail.

COURSE OUTCOMES: At the end of the Course, the Student will be able

CO1	utilize the knowledge and usage of catalysts comprising isopoly and heretopolyacids for industrial applications. [K3]
CO2	correlate and compare the properties of carboranes with that of neutral, nido, closo, aracho, hypo and conjucto boranes. [K3]
CO3	predict the geometry, shape, coordination number, magnetic properties and stability of octahedral, square planar and tetrahedral complexes predominantly of d-block elements. [K3]
CO4	know the various donor systems donating sigma and pi bonds involved in the synthesis of organometallic compounds. [K3]
CO5	distinguish the concept of stereoisomerism from structural isomerism pertaining to six and four membered inorganic complexes. [K3]

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	PO										PSO				
	1	2	3	4	5	6	7	8	9	10	1	2	3	4	5
CO1	3	3	3	3	3	3	2	2	2	3	3	3	3	3	2
CO2	2	3	3	3	3	3	2	2	2	3	3	3	3	3	2
CO3	3	3	2	3	2	3	2	2	3	3	3	3	3	3	2
CO4	3	3	3	3	2	3	3	3	3	3	3	3	3	3	3
CO5	3	3	3	3	3	3	3	3	3	3	3	3	2	3	3

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	CONTENTS OF MODULE	Hrs	COs
1	**STRUCTURE AND BONDING-I** 1.1 Poly acids: Isopolyacids and heteropolyacids of transition metals- $\{[X^{n+}M_{12}O_{40}]^{(8-n)-}$ (X= P, M= W)}, $\{[X_2^{5+}M_{18}O_{62}]^{6-}$ ((X= P, M= W)}, $[H_2(W_{12}O_{40})]^{6-}$; H_3 $PW_{12}O_{40}$. 29 H_2O; $^-$ $TeMo_6O_{24}^{6-}$; Mo_7O_{24} $^{6-}$; $PMo_{12}O_{40}$ $^{3-}$; isopolyvanadates- polymerization of CrO_4^{2-} anion. 1.2 Inorganic Polymers: Silicates-Introduction, classification of silicates-ortho silicates (*Neso*) (Ex: zircon, willemite phenacite, forsterite, olivine, and garnets);pyro silicates (*soro*) (ex: thortveitite, hemimorphite);cyclo silicates (*meta*) (ex: wollastonite, benitoite, beryl and emerald); ino silicates (*chain*) (ex: amphiboles and asbestos minerals);sheet silicates (*phyllo*) (classification-clay minerals (ex: kaolinite, pyrophyllite, talc)-white asbestos (ex: chrysotile, biotite)-micas (ex: muscovite and margarite)-montmorillonite (ex: fuller's earth, bentonite and vermiculite)-three dimensional silicate (*tecto*) (classification-feldspars-zeolites-ultramarines)-formula, structure and properties only.	**17**	**CO1**

	1.3 Polyorgano phosphazenes: Introduction-structure of cyclic trimer $(NPCl_2)_3$-pi bonding in phospho-nitrilic system-Craig and Paddock-Dewar theory-structure and bonding of tetramer $(NPCl_2)_4$ and octa methyl tetraphosphaza tetraene. 1.4 Linear polymers –phosphams-advantages of inorganic polymers. Sulphur-nitrogen compounds: Preparation, properties and Structure: S_2N_2, S_4N_4, $(SN)_x$		
2	**STRUCTURE AND BONDING II** 2.1 Boranes: classification- *closo, nido, arachno,hypo* and *conjucto*. Lipscomb's rule, Wade's rule- poly skeletal electron theory (PSEPT)-calculation of number of electron deficient bonds in polyboranes. Structure, bonding and determination of *styx* numbers and topology of boron hydrides- Diborane, hexa hydrido hexaborane anion ($B_6H_6^{2-}$), Tetraborane-10, Pentaborane-9, Pentaborane-11, Decaborane-14. Carboranes: Structural similarity with boranes- Stability of closo, nido and arachno carboranes-Preparation, structure and isomerization of $C_2B_{10}H_{12}$ (no mechanism) 2.2 Metal Clusters: Definition- Clusters containing carbonyl groups-electron count and structure of clusters-Wade Rule – Mingo's rule-Chemistry of low molecularity metal clusters (up to) trinuclear metal clusters; metal-metal multiple bonds. ($Re_2Cl_8^{2-}$, $W_2Cl_9^{3-}$, $[Cr_2Cl_2]^{3-}$, Re_3Cl_9, Cu_2 and Cr_2 acetate complexes, $Mo_2Cl_8^{4-}$ only), Chalcogenides, Chevral phases. Octahedral clusters-metal only clusters-structure and bonding only.	**18**	**CO2, CO3**
3	**THEORIES OF COORDINATION COMPOUNDS** 3.1 Crystal field theory (CFT)-d-orbital splitting (octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal geometries). Spectrochemical series- Ligand field stabilization energy -concept of weak and strong fields (paramagnetic and diamagnetic property)-spin only magnetic moment (μ_s). 3.2 Applications of CFT-origin of color of the transition metal complexes-magnetic property (magnetic moment) –applications of CFSE (crystal structure of spinels, stabilization of oxidation states, and geometry of complexes)-limitations of CFT- evidences for metal-ligand orbitals overlap, nephelauxetic effect.	**17**	**CO4**

	3.3 Molecular orbital theory and energy level diagram- octahedral complexes- (sigma donor- pi donor-pi acceptor) and tetrahedral complexes. Jahn-Teller distortion-theorem- static distortion-$t_{2g}^3e_g^1$, $t_{2g}^6e_g^3$,$t_{2g}^6e_g^1$, dynamic distortion- $t_{2g}^1e_g^0$, $t_{2g}^4e_g^2$. Flattening-elongation and consequences of Jahn-Teller distortion.		
4	**ORGANOMETALLIC CHEMISTRY** 4.1 **pi donors** Structure, bonding, modes- bonding mechanism-evidences for bonding of CO, NO, alkenes, alkynes, cyclopenta diene, carbene, and fluxional behavior. Metallocenes (general stability and reactivity)- Preparation, properties, structure and bonding –ferrocene only. 4.2 **Catalysis in Organometallic Chemistry** Catalytic mechanism in the following reactions-Hydrogenation of olefins (Wilkinson's catalyst)-Tolman catalytic loops, hydroformylation (oxo process)-acetic acid from methanol-oxidation of alkenes to aldehyde and ketones (Wacker process)-catalysis in the formation of synthesis gas (syn gas)-homologation-water gas shift reaction-synthetic gasoline (Fischer-Tropsch and Mobil process- political process), olefins polymerization (Ziegler-Natta catalyst), cyclo oligomerisation of acetylene using nickel catalyst (Reppe's catalyst), polymer bound catalysts.	**20**	**CO5**
5	**STEREO ISOMERISM OF COORDINATION COMPOUNDS** 5.1. Stereochemical aspects- Stereoisomerism in Coordination Complexes; Isomerism arising out of Ligands and Ligand Conformation (bis complexes containing ethylene diamine, propylene diamine ligands- only). 5.2. Chirality and Nomenclature of Chiral Complexes; Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD). Determination of Absolute Configuration using ORD. ($[Co(en)_3]^{3+}$, $Co(gly)_3]$ complexes only).	**18**	**CO6**

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2. F.A. Cotton and G. Wilkinson, 1988, Advanced Inorganic Chemistry - A Comprehensive Text, V. Edition, John Wiley & Sons.
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5. U. Malik, G.D.Tuli and R.DMadan 1992 Selected Topics in Inoganic chemistry,
6. A.F. Wells, - 1984, Structural Inorganic Chemistry, V. Edition, Oxford
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7. Gary Wulfsberg 2002 Inorganic Chemistry I edition.
8. Asim K. Das Fundamental concepts of Inorganic Chemistry. 2008. Vol. 1-6. II Edition. (CBS Publications)

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**CIA I**	**CIA II**	**CIA III**	**ESE**
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

Course Title: CORE PAPER III - PHYSICAL CHEMISTRY – I

Course Code	**:**	**Credits**	**: 04**
L:T:P:S	**: 4:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

Course Outcomes: At the end of the Course, the Student will be able to:

CO1	compare the thermodynamics of ideal and non-ideal solutions and gases
CO2	distinguish ideal and non-ideal solutions and the excess thermodynamic functions and apply the concept of activity and activity coefficient for non-ideal non-electrolytic solutions
CO3	explain the postulates of quantum mechanics. And they can demonstrate the application of Schrodinger wave equation for various systems such as particle in a box, particle on a ring and sphere etc. and identify the quantisation of energy in confined and microscopic systems
CO4	apply Schrodinger wave equation to quantum mechanical systems such as one dimensional harmonic oscillator and rigid rotor to deduce the expression for the energy which he can use in molecular spectroscopy. And also the application of Schrodinger wave equation to hydrogen atom and identify the radial and angular probability distribution functions to visualise and grasp the concept of various orbitals and their shapes
CO5	control and manipulate the complex reactions such as reversible, consecutive, parallel and chain reactions including explosion reactions. And also the Fast reactions such as explosions could be studied experimentally by the students using relaxation methods and flash photolysis

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	**PO**								**PSO**				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**1**	**2**	**3**	**4**	**5**
CO1	**3**	**3**	**3**	**2**	**2**	**1**	**2**	**2**	**3**	**2**	**3**	**2**	**3**
CO2	**3**	**3**	**3**	**2**	**2**	**1**	**2**	**2**	**3**	**2**	**3**	**2**	**3**
CO3	**3**	**3**	**3**	**2**	**3**	**2**	**2**	**2**	**3**	**3**	**3**	**3**	**3**
CO4	**3**	**3**	**3**	**2**	**3**	**2**	**3**	**3**	**3**	**3**	**3**	**3**	**2**
CO5	**3**	**3**	**3**	**2**	**3**	**2**	**3**	**3**	**3**	**3**	**3**	**3**	**2**

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

Sl NO	CONTENTS OF MODULE	Hrs	COs
1	**Thermodynamics I** 1.1 Partial molar properties - Partial molar free energy (Chemical potential) –Gibbs Duhem equation - Partial molar volume and partial molar heat content - their significance and determination of these quantities by method of intercepts. 1.2 Variation of chemical potential with temperature and pressure. 1.3 Thermodynamics of real gases - gas mixture – fugacity-definition - determination of fugacity - variation of fugacity with temperature and pressure	18	CO1
2	**Thermodynamics II** 2.1 Thermodynamics of ideal and non ideal binary solutions - Duhem-Margules equation - application in the distillation of ideal and non ideal solutions - azeotropic mixture - dilute solutions - excess functions for non-ideal solutions and their determination. 2.2 Choice of standard states – Concept and determination of activity and activity coefficients for non-electrolytes.	18	CO2
3	**Quantum Chemistry-I** 3.1 Quantum mechanical postulates-the Schrodinger equation 3.2 Elementary applications of Schrodinger's equation-the particle in a box (one, two and three dimensional cases)-particle on a ring- particle on a sphere	18	CO3
4	**Quantum Chemistry-II** 4.1 One dimensional harmonic oscillator and isotropic oscillator- the rigid rotor- 4.2 The hydrogen atom - the Schrodinger equation for hydrogen atom - the solution - the origin of quantum number (angular momentum and spin) - their physical significance.	18	CO4
5	**Chemical Kinetics-I** 5.1 Kinetics of complex reactions - reversible reaction, consecutive reactions, parallel reactions, chain reactions - general treatment of chain reactions. Rice Herzfeld Mechanism and explosion limits. 5.2 Study of fast reactions-relaxation methods-temperature and pressure jump methods- stopped flow and flash photolysis.	18	CO5

REFERENCE BOOKS:

1. J.Rajaram & J.C.Kuriacose,1993, Kinetics and mechanism of chemical transformations, Mac Millon India Ltd.
2. K.J.Laidler, 1987, Chemical kinetics, Harper and Row, New York
3. P.W.Atkins, 1990, Physical Chemistry, Oxford
4. W.J.Moore, 1972, Physical Chemistry, Orient Longman, London
5. R.G.Frost and Pearson,1981, Kinetics and mechanism, Wiley, New York
6. S.Glasstone, 1960, Thermodynamics for chemists, Affiliated East West Press, New Delhi
7. J.Rajaram & J.C.Kuriacose, 1986, Thermodynamics for students of chemistry, Lal Nagin
8. Chand, New Delhi
9. N. Levine, Quantum Chemistry, 6th edition.
10. Quantum Chemistry, Second Edition, Donald A. McQuarrie
11. Physical Chemistry: Robert G. Mortimer

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**CIA I**	**CIA II**	**CIA III**	**ESE**
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

SYLLABUS FOR SECOND SEMESTER

COURSE TITLE: CORE IV – ORGANIC CHEMISTRY - II

Course Code	**: 1923204**	**Credits**	**: 04**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

On taking this course the student will be able to explain the basic concepts of addition reaction to carbon carbon multiple bond and elimination reaction. The student can classify and interpret mechanism of some of the important rearrangements in organic chemistry. The last part of the course will enable the student to describe the salient features of oxidation and reduction reactions in organic synthesis. (Stereochemical aspects to be studied wherever applicable)

COURSE OUTCOMES: At the end of the Course, the Student will be able to:

CO1	Demonstrate the knowledge to understand and generate ideas about addition to carbon – carbon and carbon hetero multiple bond reactions. (K3)
CO2	Develop knowledge about reactions involving carbon –carbon and carbon hetero multiple bonds (K3)
CO3	Illustrate the basic principle and application of elimination reactions (K4)
CO4	Demonstrate the ability to distinguish between different types of molecular rearrangements and apply their importance in organic reaction mechanisms. (K4)
CO5	Assess various oxidation and reduction reactions and appreciate their importance in organic synthesis. (K4)

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	**PO**										**PSO**				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	2	2	2	3	2	2	2	3	3	3	3	3	2
CO2	3	3	2	2	2	3	2	2	2	3	3	3	3	3	2
CO3	3	3	3	2	2	3	2	3	2	3	3	3	2	3	2
CO4	3	3	3	2	2	3	2	2	2	3	3	3	2	3	2
CO5	3	3	3	3	2	3	3	3	2	3	3	3	2	3	2

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	CONTENTS OF MODULE	Hrs	COs
1	**ADDITION TO CARBON-CARBON AND CARBON-HETERO ATOM MULTIPLE BONDS I** 1.1 Addition of Halogen and halogen acids to multiple bonds – syn and anti addition. 1.2 Hydration of Olefins and acetylenes 1.3 Hydroboration – reaction with alkaline hydrogen peroxide – 1.4 Hydroxylation using OsO_4, $KMnO_4$ and alkaline hydrogen peroxide, peracids 1.5 Prevost and Woodward modifications 1.6 Michael Addition – dimethyl copper mediated addition-preparation of precursor for Robinson Annulation reaction – Regio chemistry.	**18**	**CO1**
2	**ADDITION TO CARBON-CARBON AND CARBON-HETERO ATOM MULTIPLE BONDS II** 2.1 Addition of carbenes and nitrenes -methods of generation and addition to double bonds, Simmon-Smith Reaction. 2.2 Diels Alder Reaction and 1, 3-dipolar additions - stereo electronic effects – use of Lewis acids, Alder's endo rule - Regio chemistry and retro Diels Alder reaction. 2.3 Mannich reaction, Stobbe and Darzen reactions - Knovenegal condensation, Benzoin condensation. 2.4 Ylides - N, O, S - Phosphorous ylides - Wittig reaction - mechanism and applications; S-ylides- Jacobson–Corey–Chaykovsky reaction -Difference in the reactivity of P and S ylides with carbonyl compounds. 2.5 Difference in the reactivity of dimethyl- and dimethoxysulphoniummethylides with ὰ,β- unsaturated carbonyl compounds, cyclohexanones and norbornyl systems(exo- and endo- additions)	**18**	**CO2**
3	**ELIMINATION REACTIONS** 3.1 Types - E_1, E_2, Ei and E_1cB mechanism –Factors influencing the eliminations – substitution/elimination ratio- E_1/E_2 ratio- Orientation of the double bond -Hoffman and Saytzeff rule -	**18**	**CO3**

	Factors influencing Hoffman and Saytzeff products- syn and anti elimination with examples. E1, E2 and E1cB spectrum , MoreO'Ferral diagram 3.2 Competition between elimination and substitution, orientation of product formation, Stereochemistry of E2 eliminations in cyclohexane systems. 3.3 Typical eliminations to be studied - dehydration, dehydro-halogenation – dehalogenation- 3.4 Mechanism of pyrolytic eliminations. Examples: Chugaev and Cope Elimination.		
4	**MOLECULAR REARRANGEMENTS** 4.1 Classification of molecular rearrangements based on migrating centre. I. Nucleophilic Rearrangement (Anionotropic/Carbonium ion Rearrangement) II. Electrophilic rearrangement Cationotropic/Carbanion Rearrangement) 4.2 Rearrangements involving migration to electron-deficient carbon Demjanov Rearrangement, dienone-phenol, Benzil - Benzilic acid Rearrangement Wolff Rearrangement 4.3 Rearrangements involving migration to electron rich carbon: Favorskii Rearrangement, Neber Rearrangement, Stevens, Wittig, Sommelet 4.4 Rearrangements involving migration to electron deficient nitrogen: Beckmann Rearrangement 4.5 Rearrangements involving migration to electron deficient oxygen: Baeyer-Villiger Rearrangement, Dakin, Fries , Claisen, Benzidine	**18**	**CO4**
5	**OXIDATION AND REDUCTION** 5.1. Mechanism and study of the following oxidation reactions: Oxidation of alcohols - using Chromium based reagents - PCC, PDC, Jones reagent – Mechanism of oxidation of alcohols using DMSO activated with electrophiles such as DCC, oxalyl chloride, acetic anhydride & SO_3 - Pfitzner Moffatt and Swern oxidation – Sharpless Epoxidation using peracids-hydroxylation of olefins using OsO_4 (both cis and trans), cleavage of 1,2-glycols using	**18**	**CO5**

	periodate, lead tetra acetate- Ozonolysis. 5.2. Allylic oxidation of olefins using SeO_2 - oxidation of methylene to carbonyl (Riley reaction) -oxidation of aryl methanes (Etard reaction) 5.3. Synthetic importance of Clemmensen and Wolf-Kishner reductions- Modifications of Wolf-Kishner reduction-Birch reduction, MPV reduction. Reduction with $NaBH_4$, $LiAlH_4$, $Li(tBuO)_3$, AlH_3, DIBAL-H, Selectivity in reduction of 4-t-butyl cyclohexanone using selectrides		

TEXTBOOKS:

1. Bruckner R. Advanced Organic Chemistry, Reaction Mechanism, Elsevier, New Delhi, 2002.
2. Carey F.A. and Sundberg R.J., Advanced Organic Chemistry, Part A and Part-B, 4th Edition, Plenum Press., New York, 2001.
3. March J., Advanced Organic Chemistry, 4th Edition, John Wiley & Sons Singapore, 2002.

REFERENCE BOOKS:

1. Gilchrist T.L. and Rees C.W., Carbenes, Nitrenes and Arynes, Thomas Nelson and Sons Ltd., London, 1969.
2. Carruthers W., Some Modern Methods of Organic Synthesis, 3rd Edition Cambridge University Press, 1993
3. House H.O., Modern Synthetic Reactions, The Benjamin Cummings Publishing Company, London, 1972.
4. March J. and Smith M.B., March's Advanced Organic Chemistry: Reactions, Mechanisms and structure, 6th edition, Wiley, 2007.
5. Jonathan Clayden, Nick Greeves & Stuart Warren, Organic Chemistry, Second Edition, Oxford University press, 2012.

WEBSITES:

1. http :// info dome . sdsu, ./research/ guides/ science/ org chemistryblr. Html
2. http :// www.liv.ac.uk/chemistry/links /reactions.html
3. http ://orgchem.chem..uconn.edu/namereact/named.html
4. www.gcocities.com/ chempen softwar4ee/reactions.html

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**CIA I**	**CIA II**	**CIA III**	**ESE**
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

COURSE TITLE: CORE V – INORGANIC CHEMISTRY – II

Course Code	**: 1923205**	**Credits**	**: 04**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVE:

This paper explains the basic concepts of the role of elements involved in the active metabolism of human kind. The role of essential, trace and need of elements in the biomineralisation, transportation, storage with respect to Fe, Cu, and Zn is provided in detail in order to understand the essence and role of elements in our daily life as enzymes or cofactors. A broad picture on the role of elements involved in electron transfer, energy transfer and photosynthesis is provided. The concept and idea of Solid state chemistry and its application in material chemistry is explained as illustrative concepts linked to semiconductors, solid state lasers, phosphors, superconductors, alloys and solid melt solutions. A conceptual idea and a fundamental aspect on the electronic spectroscopy on the study of the inner core electrons is provided in the form of photoelectron spectroscopy which is explained with examples ranging from simple homonuclear and heteronuclear molecules.

COURSE OUTCOMES: At the end of the Course, the Student will be able

CO1	To assess the role of metal ions, metallo enzymes and Vitamins in human body and other living organisms (K3, K5)
CO2	To illustrate the role of transport proteins, study of photosynthesis, nitrogen fixation and anti cancer activity (K4)
CO3	Interpret of XPES, UPES and evaluation of ionisation potential and chemical identification of elements. (K3)
CO4	To determine the effect of Magnetic Behavior, magnetic susceptibility and its applications (K3)
CO5	To examine the related applications of X-Ray, Neutron and Electron Diffraction, and solid electrolytes and solid solutions (K4)

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	PO										PSO				
	1	2	3	4	5	6	7	8	9	10	1	2	3	4	5
CO1	3	2	3	3	3	3	3	2	2	3	3	3	3	3	2
CO2	3	2	2	3	3	3	2	2	2	3	3	3	3	3	2
CO3	3	2	3	2	3	3	2	2	2	3	3	2	3	3	2
CO4	3	2	3	2	3	3	2	2	2	3	3	2	3	3	2
CO5	3	2	2	2	3	3	3	3	2	3	3	2	3	3	2

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	CONTENTS OF MODULE	Hrs	COs
1	**BIO INORGANIC CHEMISTRY-I** 1.1 Iron proteins involved in transport and storage of iron-ferritin-bio mineralization-structural features -apoferritin-structural features-hemosiderin-transferrin-role of synergistic anion ligand (carbonate)-stability of Fe (III) chelate. 1.2 Iron transport in lower organisms-siderophores-definition-iron binding groups-classification. 1.3 Sodium and potassium pump-transport processes- role of Mg^{2+} ions-conformational states E1 and E2-selectivity of the pump. 1.4 Bio elements and their classification in human body-bio elements and their role in human body-Na, K, Mg, Ca, P, Fe, Cu, Zn, I, F, Co, Mn-role of coordination complexes in living body. 1.5 Metallo enzymes – apo enzymes-co enzymes-co factor-zinc enzymes – structure, function and mechanism of carboxy peptidase A (CPA) and carbonic anhydrase (CA). 1.6 Vitamin B_{12}- unusual aspects of cobalamine-structural features of vitamin B_{12}-different forms of cobalamine- chemistry of cobalmine- oxidation state of Cobalt in cobalmine- electrophilic and nucleophilic character of coblamine- properties of Co-C bonds in cobalamine in terms of bond fission-special characteristics of vitamin B_{12} coenzyme.	**15**	**CO1**

	1.7 Function and structural features of Catalase and peroxidase. Copper proteins: Classification-Type I- structural differences-plastocyanin- stellacyanin-azurin. Type II, Type III-its biological role.		
2	**BIO INORGANIC CHEMISTRY-I I** 2.1 Transport proteins, Oxygen carriers – haemoglobin – myoglobin – structure, co-operativity and Bohr effect- Perutz mechanism–role of protein-Picket-Fence model. Biological redox systems: Cytochromes – structure and classification. Cytochrome P450-structural features-functions and mechanism of activity. 2.2 Iron sulphur proteins – general features of Fe-S proteins-Rubredoxin –Ferredoxin (Fd)-4Fe-4S (Fd), Rieske centre-2Fe-2s (Fd), 3Fe-4S (Fd), 8Fe-8S (Fd). 2.3 Chlorophylls and Photosynthesis-light phase and dark phase reactions in photosynthesis-chlorophyll-structural features-role of Mg^{2+} in chlorophyll-electron transport chain in light phase reactions of photosynthesis Z-scheme-water splitting reaction catalysed by Mn-protein in photosynthesis. 2.4 Nitrogen fixation - introduction, nitrification and de-nitrification-fundamental features-in vitro nitrogen fixation-in vivo nitrogen fixation-structural features-Fe protein-Fe Mo cofactor. 2.5 Anti cancer activity of Platinum complexes, Mechanism of anticancer activity of cis-DDP, non-activity of trans-DDP. Only examples of anticancer metal complexes (other than Pt-complexes). Radio isotopes – diagnosis and treatment.	**20**	**CO2**
3	**PHOTO ELECTRON SPECTROSCOPY** 3.1 Theory of X-ray Photo Electron Spectroscopy (XPES), Ultra Violet Photo Electron Spectroscopy (UVPES)-evaluation of ionisation potential-chemical identification of elements. 3.2 Electronic spectra for chemical analysis (ESCA)- Koopman's theorem-chemical shift-UPES of ammonia, molecular nitrogen, molecular oxygen, carbon monoxide, water and hydrogen chloride. Hydrogen molecule, magnesium oxide, ethyl trifluoroacetate and nitrosonium ion. 3.3 Vibrational fine structure and their origin-evaluation of vibrational constants from UPES-spin-spin coupling-spin orbit coupling.	**15**	**CO3**
4	**SOLID STATE CHEMISTRY – I** 4.1 Types of Magnetic Behaviour - Diamagnetism, Paramagnetism, Ferromagnetism, Anti-ferromagnetism and Ferrimagnetism.	**20**	**CO4**

	Orbital momentum, spin momentum, spin-orbit coupling-effective magnetic moment (μ_{eff})- determination of μ_{eff} - comparison of Co^{2+} and Ni^{2+} octahedral and tetrahedral complexes. Hysterisis (hard magnets and soft magnets). 4.2 Magnetic susceptibility-Determination of magnetic susceptibility by Guoy method and Faraday methods-applications of magnetic susceptibility. 4.3 Spinels and inverse spinels (Problems). Solid State Lasers-ruby laser-Nd lasers, Inorganic Phosphors and Garnets.		
5	**SOLID STATE CHEMISTRY –II** 5.1. Comparison of X-Ray, Neutron and Electron Diffraction-applications. 5.2. Superconductors - BCS theory, Cooper pairs. 5.3. Solid electrolytes-beta alumina-AgI and Ag^+ ion solid electrolytes-halide ion conductors-oxide ion conductors-applications of solid electrolytes. Reactions in Solid State-Diffusion Coefficient, Diffusion Mechanisms, Vacancy and Interstitial Diffusion. 5.4. Solid Solutions: substitutional solid solutions-interstitial solid solutions. Phase transitions-reconstructive and displacive transitions-thermodynamic classification of phase transitions. **5.5.** Crystal chemistry and phase transitions-Martensitic transformations-order disorder transitions- Super Structure.	**20**	**CO5**

TEXT BOOKS:

1. K.F. Purcell and J.C. Kotz, 1977, Inorganic Chemistry WB Saunders Co., U.S.A.
2. J.E. Huheey, 1993, Inorganic Chemistry, IV Edition, Harper and Collins, NY.
3. F.A. Cotton and G.W. Wilkinson, 1988, Advanced Inorganic Chemistry - A Comprehensive Text; John Wiley & Sons.
4. B.E. Dogulas. D Mc Daniels and Alexander, 1983, Concepts and Models of Inorganic Chemistry, Oxford IBH.
5. A.R. West, 1991, Basic Solid State Chemistry, John Wiley.
6. W.E. Addison, 1961, Structural Principles in Inorganic Chemistry, Longman.
7. M. Adams, 1974, Inorganic Solids, John Wiley Sons.
8. K.Hussain, Reddy Bio Inorganic Chemistry, New Age International Pvt., Ltd.,
9. Williams D.R., Introduction to Bio Inorganic Chemistry

10. Fiabre F.M. and Williams D.R The Principles of Bio Inorganic Chemistry Royal Society of Chemistry – Monograph for teachers.
11. G. N. Mugherjee and Arabinda Das 1993. Elements of Bio Inorganic Chemistry.
12. M. Satake and Y. Mido -1996 Bio Inorganic Chemistry Discovery publishing House New Delhi.
13. Asim K Das-2011 Bio Inorganic Chemistry Books and Allied Private Ltd.
14. Advanced Inorganic Chemistry Vol I and II by S. P. Banerjee. Books and Allied (P) Ltd. 2003.
15. E. A. V. Ebsworth, D.W.H. Rankin and S. Cradock, Structural Methods in Inorganic Chemistry, Blackwell Scientific Publ., 1976.
16. Basic Organometallic Chemistry: Concepts, Syntheses and Applications 2nd Edition, by B. D. Gupta and A. J. Elias, University Press.

REFERENCE BOOKS:

1. S.F.A. Kettle, 1973, Coordination Chemistry, ELBS.
2. B.N. Figgis, 1966, Introduction to Ligand Fields, Interscience.
3. M.N. Hughes, 1982, The Inorganic Chemistry of Biological processes, II Edition, Wiley London
4. M.C. Shrivers, P W. Atkins, CH Langford, 1990, Inorganic Chemistry, OUR
5. M.C. Day and J. Selbin, 1974, Theoretical Inroganic Chemistry, Van Nostrand Co., NY.
6. A.F. Wells, - 1984, Structural Inorganic Chemistry, V. Edition, Oxford
7. A.R. West, 1990, Solid State Chemistry, John Wiley.
8. K. Burger, 1973, Coordination Chemistry, Experimental methods, Butterworths.
9. C.N.R. Rao, J.R. Ferraro, 1970, Spectroscopy in Inorganic Chemistry, Vol. I and Vol. II, Academic Press.
10. G. Aruldas, Molecular Structure and Spectroscopy, Prentice Hall.
11. G.Eicharn, 1973 Inorganic Bio Chemistry volume I &II Elsevier
12. Bertini, Gray, Lippard, Valentine –1998 Bio Inorganic Chemistry South, Asian Edition

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**CIA I**	**CIA II**	**CIA III**	**ESE**
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

COURSE TITLE: CORE VI - PHYSICAL CHEMISTRY – II

Course Code	**: 1923206**	**Credits**	**: 04**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVE:

To learn the fundamentals and applications of Group theory in chemistry and approximation methods of quantum chemistry, reactions in solutions, enzyme catalysis and theories of adsorption.

COURSE OUTCOMES: At the end of the Course, the Student will be able:

CO1	To paraphrase the fundamentals and applications of Group theory. [K2]
CO2	To articulate group theory to molecules and predict IR and electronic spectra. [K3]
CO3	To compute approximation methods to the atoms of more than one electron. [K3]
CO4	To predict the effect of temperature on the rate of reaction. [K2]
CO5	To employ enzyme catalysis and adsorption for practical situations.[K3]

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	**PO**										**PSO**				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	3	3	3	3	2	2	2	3	3	3	3	3	2
CO2	2	3	3	3	3	3	2	2	2	3	3	3	3	3	2
CO3	3	3	2	3	2	3	2	2	3	3	3	3	3	3	2
CO4	3	3	3	3	2	3	3	3	3	3	3	3	3	3	3
CO5	3	3	3	3	3	3	3	3	3	3	3	3	2	3	3

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	CONTENTS OF MODULE	Hrs	COs
1	**GROUP THEORY IN CHEMISTRY-I** 1.8 Definition of group - Symmetry elements and symmetry operations 1.9 Point groups-identification and determination-reducible and irreducible representations Direct product representation 1.10 Orthogonality theorem and its consequences-character table	18	CO1
2	**GROUP THEORY IN CHEMISTRY-I I** 2.1 Hybrid orbital in non-linear molecules (CH4, XeF4, BF3, SF6 and NH3). 2.2 Determination of representations of vibrational modes in non-linear molecules (H2O, CH4, XeF4, BF3, SF6 and NH3) 2.3 Symmetry selection rules for infrared, Raman and electronic Spectra-Mutual exclusion principle 2.4 Electronic Spectra of Ethylene and formaldehyde-SALC method of constructing MOs of water, ammonia, cyclobutadiene and benzene	18	CO2
3	**QUANTUM CHEMISTRY-III** 3.1 Approximation methods: Variation method- application to Particle in one dimensional box, hydrogen atom, helium atom 3.2 Time independent Perturbation method- Application to Particle in one dimensional box, anharmonic oscillator, hydrogen atom (stark effect) and helium atom 3.3 Time dependent perturbation theory – Selection rules for transitions. 3.4 Pauli principle, Spin function, Anti-symmetric wavefunction – Slater determinants, Slater orbital and HF-SCF methods. R. S. Coupling and term symbols for atoms in the ground state	18	CO3
4	**CHEMICALKINETICS-II** 4.1 Transition state theory 4.2 Reactions in solutions, effect of pressure, dielectric constant and ionic strength on reactions in solutions 4.3 Kinetic isotope effects-linear free energy relationships-Hammett and Taft equations.	18	CO4

	4.4 Acid base catalysis-Bronsted catalysis law		
5	**CHEMICALKINETICS-III** 5.1. Catalysis by Enzymes: Rate of enzyme catalyzed reactions, effect of substrate concentration, pH and temperature on enzyme catalyzed reactions-inhibition of enzyme catalyzed reactions. 5.2. Adsorption: Langmuir and BET adsorption isotherms-adsorption coefficient and its significance 5.3. Kinetics and mechanism of surface reactions-catalysis by metals, semiconductor oxides.	18	CO5

REFERENCE BOOK:

1. J.Rajaram & J.C.Kuriacose, 1993, Kinetics and mechanism of chemical transformations, Mac Millon India Ltd.
2. K.J.Laidler, 1987, Chemical kinetics, Harper and Row, New York
3. P.W.Atkins, 1990, Physical Chemistry, Oxford
4. W.J.Moore, 1972, Physical Chemistry, Orient Longman, London
5. R.G.Frost and Pearson,1981, Kinetics and mechanism, Wiley, New York Chand, New Delhi
6. K.V.Raman, 1990, Group Theory and its applications to chemistry, Tata Mc.Graw Hill 7. F.A.Cotton, 1971, Chemical applications of Group Theory, John Wiley and Sons Inc., New York
7. S. Swarnalakshmi, T. Saroja and R. M. Ezhilarasi, 2008, A simple approach to Group theory in chemistry, University Press
8. N. Levine, Quantum Chemistry, 6th edition.
9. Quantum Chemistry, Second Edition, Donald A. McQuarrie 13. Physical Chemistry: Robert G. Mortimer.

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**CIA I**	**CIA II**	**CIA III**	**ESE**
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

COURSE TITLE: CORE VII - ORGANIC CHEMISTRY PRACTICALS I

Course Code	**: 1923207**	**Credits**	**: 04**
L:T:P:S	**: 0:0:6:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

On taking this course, the students will be able to

I. *Analyse and separate organic mixture and Identify the components in a two-component mixture and prepare derivatives and determine the melting point of individual components.*

II Apply the lab techniques in analysis of organic compounds.

III. *Prepare simple organic compounds involving one and two stages and determine their yield.*

COURSE OUTCOMES:

At the end of the Course, the Student will be able to:

CO1	Demonstrate the knowledge to separate a given binary or tertiary organic mixture and analyse the compounds present in it. (K3)
CO2	Design and proceed with single stage and two stage preparation of organic compounds employing the principles which they learnt in the theory during this year of study.(K3)
CO3	Apply the principles of green synthesis and prepare simple organic compounds (K4)

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	**PO**										**PSO**				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	2	3	2	3	2	3	2	3	3	3	3	3	3
CO2	3	3	2	3	2	3	2	2	2	3	3	3	3	3	3
CO3	3	3	2	3	2	3	2	2	3	3	3	3	3	3	3

S. No.	CONTENTS OF MODULE	COs
1.	**Preparation involving single step:** 1. 1, 2, 3, 4-Tetrahydrocarbozole from cyclohexanone 2. p-chlorotoluene from p-toluidine 3. Preparation of dibenzylideneacetone from benzaldehyde 4. Preparation of benzylidene acetophenone from benzaldehyde (Chalcone) 5. Reduction - Benzhydrol from benzophenone 6. Pinacol-Pinacolone rearrangement from Pinacol hydrate 7. 7. Fischer Indole synthesis from cyclohexanone	**CO1**
2.	**Preparations from the following involving two stages:** 1. 2, 4-Dinitrobenzoic acid from p-nitro toluene. (Oxidation /Aromatic electrophilic substitution) 2. 2-4, Dinitrophenyl hydrazine from p-nitrochlorobenzene. (Aromatic electrophilic and Nucleophilic substitution) 3. Preparation of Acetanilide from Acetophenone	**CO2**
3.	**Green synthesis** *Bromination of acetanilide using ceric ammonium nitrate.	**CO3**

***Not for exam**

RERERENCES:

1. Arthur I. Vogel A Text Book of Practical Organic Chemistry
2. Raj . K. Bansal, Laboratory Manual of Organic Chemistry, Wiley Eastern Limited.
3. Mann & Saunders, Laboratory Manual of Organic Chemistry.

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**MODEL**	**ESE**
Marks (out of 50)	**60**	**60**
Remember		
Understand		
Apply	30	30
Analyze	30	30
Evaluate		
Create		

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	
Understand	
Apply	50
Analyse	50
Evaluate	
Create	

COURSE TITLE: CORE VIII - INORGANIC CHEMISTRY PRACTICALS I

Course Code	**: 1923208**	**Credits**	**: 04**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

This comprises of TWO parts

I. Analysis of inorganic mixture. The course is designed to enable students to have an exposure to lab techniques in analysis of inorganic compounds containing a combination of rare and common cations. The concept of solubility product, common ion effect and the role of oxidizing and reducing agents in determination of two common actions and two less common actions is provided through semi micro qualitative analysis.

II. Estimation of Mg, Zn and Ca using EDTA by complexometric titration and estimation of Fe by Cerimetry.

COURSE OUTCOMES: At the end of the Course, the Student will be able to**:**

CO1	To provide an insight into the role of EDTA in complexometric titrations and its significance in the quantitative estimation of Ca, Mg and Zn.
CO2	This technique enables the student to carry out an idea about the technique and mechanism of determination of the presence of dissolved metal salts in water.
CO3	Industrial application of the analysis of water is imparted to the students to excel in industrial and research labs
CO4	The students are taught with the technique and elementary idea of detection of metals as common and rare cations in a mixture.
CO5	The students are able to qualitatively identify several cations based on the knowledge of solubility product, ionic product and precipitating agents.
CO6	Identification of metals using spot reagents is of analytical importance to the students who can apply these techniques in food processing labs and dairy products.

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	PO										PSO				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	3	3	2	3	2	2	2	3	3	3	3	3	2
CO2	3	3	2	3	2	3	2	2	2	3	3	3	3	3	2
CO3	3	3	3	3	2	3	2	3	2	3	3	3	2	3	2
CO4	3	3	2	2	2	3	2	2	2	3	3	3	2	3	2
CO5	3	3	2	3	2	3	2	2	2	3	3	3	3	3	2
CO6	3	3	3	3	2	3	2	3	2	3	3	3	2	3	2

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	CONTENTS OF MODULE	COs
1	Semi micro qualitative analysis of mixtures containing two common and two rare cations. The following are the rare cations to be included: W, Mo, Ti, Te, Se, Ce, Th, Zr, V, U and Li.	**CO1, CO2, CO3, CO4**
2	Volumetric estimations 1. Complexometric titrations (EDTA) – Estimation of Ca, Mg and Zn 2. Cerimetry – Estimation of iron using ferroin indicator	**CO5, CO6**

TEXT BOOKS:

1. Vogel, Text book of Inorganic quantitative analysis.
2. Dougles A. Skoog, Principles of Instrumental Analysis, 3rd Edition.
3. Inorganic semimicro qualitative analysis,V.V. Ramanujam,The National publishing company , Ed:3 ,2007

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**MODEL**	**ESE**
Marks (out of 50)	**60**	**60**
Remember		
Understand		
Apply	30	30
Analyze	30	30
Evaluate		
Create		

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	
Understand	
Apply	50
Analyse	50
Evaluate	
Create	

ELECTIVE I
COURSE TITLE: PHYSICAL CHEMISTRY PRACTICALS I

Course Code	**: 1923209**	**Credits**	**: 03**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

To understand and verify the concepts and equations in physical chemistry by carrying out the following suitable experiments.

COURSE OUTCOMES: At the end of the Course, the Student will be able to

CO 1	To verify the isotherm equation. (exp.1)
CO 2	To interpret the various phases in binary and ternary system. (exp 2,3,4)
CO 3	To determine the equilibrium constant, concentration, molecular weight by partition method. (exp 5,6,7)
CO 4	To assess the zero, first, second order kinetics of the reaction volumetrically(exp 8,9,11,13,17)
CO 5	To assess the first order kinetics of the reaction conductometrically (exp 10 ,12)
CO 6	To understand partial molar properties in binary mixture (exp 15,16)
CO 7	To determine the specific rotation and concentration of the non -electrolyte polarimetrically.(exp 18.19)
CO 8	To verify the Bronsted Bjerum equation or effect of salt in kinetics of the reaction. (exp 17, 20)

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	**PO**										**PSO**				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	3	3	2	3	2	2	2	3	3	3	3	3	2
CO2	3	3	2	3	2	3	2	2	2	3	3	3	3	3	2

CO3	3	3	3	3	2	3	2	3	2	3	3	3	2	3	2
CO4	3	3	2	2	2	3	2	2	2	3	3	3	2	3	2
CO5	3	3	2	3	2	3	3	3	2	3	3	3	2	3	2
CO6	3	3	2	2	2	3	2	2	2	3	3	3	2	3	2
CO7	3	3	2	3	2	3	3	3	2	3	3	3	2	3	2
CO8	3	3	2	3	2	3	3	3	2	3	3	3	2	3	2

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	**LIST OF EXPERIMENTS**	**COs**
1	Study of the adsorption of acetic acid or oxalic acid on charcoal, verification of Freundlich Isotherm and determination of concentration of given acetic acid or oxalic acid.	**CO1**
2	Construction of phase diagram for a simple binary system forming Eutectic mixture;naphthalene – biphenyl, naphthalene –p-dichlorobenzene, naphthalene-diphenylamine.	**CO2**
3	Construction of phase diagram for a simple binary system forming Compound.	**CO2**
4	Construction of phase diagram for the three component system (partially miscible liquid system) Chloroform –aceticacid – water. Construction of phase diagram of Nicotine –water system.	**CO2**
5	Determination of the equilibrium constant of the reaction between iodine and potassium iodide by partion method.	**CO3**
6	Determination of the concentration of given potassium iodide solution by partition method.	**CO3**
7	Determination of molecular weight of benzoic acid in benzene and the degree of association of benzoic acid in benzene using partition method.	**CO3**
8	Kinetic study and comparison of rate constant for the inversion of cane sugar in presence of acid using polarimeter.	**CO4**
9	Kinetic study of the reaction between acetone and iodine in acidic medium and determination of the order with respect to iodine and acetone.	**CO4**

10	Kinetic study of saponification of ethylacetate by sodium hydroxide conductometrically and determination of order of the reaction.	**CO5**
11	Kinetic study and comparison of acid strengths using acid catalysed hydrolysis of methyl acetate.	**CO4**
12	Determination of temperature coefficient and energy of activation for the acid catalysed hydrolysis of methylacetate.	**CO5**
13	Determination of the rate constant and order for the reaction between potassium persulphate and potassium iodide	**CO4**
14	Study of the primary salt effect on the kinetics of oxidation of iodide by persulphate.	
15	Determination of partial molar volume of a binary solvent mixture.	**CO6**
16	Study of variation of viscosity of a binary solvent mixture.	**CO6**
17	Kinetic study and effect of solvent on acid catalysed hydrolysis of methyl acetate.	**CO8**
18	Determine the specific rotation of camphor in benzene and carbon tetrachloride by polarimetry.	**CO7**
19	To Determine the percentage of two optically active substances (d-glucose & d tartaric acid) in a mixture polarimetrically	**CO7**
20	Study the effect of addition of an electrolyte on solubility of an organic acid	**CO8**

Note: A minimum of 10 – 12 experiments have to be performed.

REFERENCE BOOK:

1. Physical Chemistry Laboratory manual Branch IV Chemistry compiled by Dr. B. Viswanathan
2. Dr. V. R. Vijayaraghavan, Dr. T. Sundaravelu, Dr. Kamala Govindarajan, Dr.S.Vivekanandn and Dr. V. Kannappan Centre for Science Education School of Chemistry, University of Madras
3. Findley's practical physical chemistry, 9th edition,revised by B.P.Levitt
4. Experiments in physical chemistry, carl garland, Joshep Niber, David shoemaker
5. Physical Chemistry Practical Manual I – compiled by Dr. S. Bangaru Sudarsan Alwar, Dr. C. Srinivasan, Mr. R. Ramesh Kumar and Mr. V. Rajagopalan, P.G. & Research Department of Chemistry, D. G. Vaishnav College, Arumbakkam, Chennai 600106.

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**MODEL**	**ESE**
Marks (out of 50)	**60**	**60**
Remember		
Understand		
Apply	30	30
Analyze	30	30
Evaluate		
Create		

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	
Understand	
Apply	50
Analyse	50
Evaluate	
Create	

ELECTIVE PAPER I

COURSE TITLE : ADVANCED QUANTUM MECHANICS FOR COMPUTAIONAL CHEMISTRY

Course Code	**:**	**Credits**	**: 03**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVE:

To learn the advances in quantum mechanics like slater determinants, Hartee Fock approximation, Configuration Interaction , Pair and Coupled-Pair Theories and Many-Body Perturbation Theory.

COURSE OUTCOMES: At the end of the Course, the Student will be able:

CO1	To paraphrase the many electron wave functions, spin orbitals and spatial orbitals. [K4]
CO2	To articulate quantum mechanics to the Coulomb and exchange operators, –the Fock Operator. [K4]
CO3	To compute approximation methods to truncated configurational interactions and the Size-Consistency Problem. [K3]
CO4	To predict the Coupled – Pair Theories and Many – Electron Theories with Single particle Hamiltonians [K3]
CO5	To illustrate Rayleigh-Schrodinger Perturbation theory and Orbital perturbation theory [K2]

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	**PO**										**PSO**				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	3	3	3	3	2	2	2	3	3	3	3	3	2
CO2	2	3	3	3	3	3	2	2	2	3	3	3	3	3	2
CO3	3	3	2	3	2	3	2	2	3	3	3	3	3	3	2
CO4	3	3	3	3	2	3	3	3	3	3	3	3	3	3	3
CO5	3	3	3	3	3	3	3	3	3	3	3	3	2	3	3

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	CONTENTS OF MODULE	Hrs	COs
1	**UNIT -1: MANY ELECTRON WAVE FUNCTIONS:** 1.1 – The electronic problem: Atomic units – The Born-Oppenheimer Approximations – The Antisymmetry or Pauli Exclusions Principle 1.2 – Orbitals, Slater Determinants and Basis Functions: Spin Orbitals and Spatial orbitals - Hartree Products – Slater determinants – Hartree Fock approximation – The Minimal Basis H_2 model – Excited Determinants	**18**	CO1
2	**UNIT -2: THE HARTREE-FOCK APPROXIMATION** 2.1 – The Hartree-Fock Equations: The Coulomb and Exchange Operators – The Fock Operator 2.2 – Restricted Closed – Shell HF: The Roothan Equations\ Model Calculations on H2 and HeH^+ - Polyatomic basis Sets 2.3 – Unrestricted Open – Shell Hartree – Fock	18	CO2
3	**UNIT -3: CONFIGURATION INTERACTION** 3.1. – Multiconfigurational wave functions and the structure of the Full CI Matrix 3.2 – Doubly excited CI 3.3 – The Multiconfiguration Self- Consistent Field and Generalized Valence Bond Methods 3.4 – Truncated CI and the Size-Consistency Problem	18	CO3
4	**UNIT -4: PAIR AND COUPLED-PAIR THEORIES** 4.1 – The Independent Electron pair Approximation 4.2 - Coupled – Pair Theories 4.3 – Many – Electron Theories with Single particle Hamiltonians	18	CO4
5	**UNIT -5: MANY-BODY PERTURBATION THEORY** 5.1 – Rayleigh-Schrodinger Perturbation theory 5.2 – Orbital perturbation theory 5.3 – Perturbation Expansion of the Correlation Energy 5.4 – Diagrammatic representation of the perturbation expansion of the Correlation Energy	18	CO5

SUGGESTED REFERENCE BOOKS:

1. N. Levine, Quantum Chemistry, 6th edition.
2. Quantum Chemistry, Second Edition, Donald A. McQuarrie 13. Physical Chemistry: Robert G. Mortimer.
3. Quantum Chemistry, Second Edition, Donald A. McQuarrie

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**CIA I**	**CIA II**	**CIA III**	**ESE**
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

ADVANCED COURSE I

COURSE TITLE: ANALYTICAL CHEMISTRY PRACTICALS I

Course Code	**: 1923210**	**Credits**	**: 03**
L:T:P:S	**: 4:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVE:

This course aims to demonstrate the basic analytical concepts involving instrumentation with the aid of appropriate experimental procedure. In addition, this course also focuses on the quantitative determination of samples under investigation and makes use of statistical tools to assess the precision and accuracy of the entities in detail.

COURSE OUTCOMES: At the end of the Course, the Student will be able to:

CO1	Prepare solution of any sort of the commonly used parameters. Molarity, molality, normality, w/v, v/v, ppm and ppb.
CO2	Analyze based on the statistical tools like t-test, Q-test etc.
CO3	Demonstrate t-test as hypothesis testing tool, which allows testing of an assumption applicable to a population.
CO4	Analyze on the precision and accuracy of the data obtained from the experiment.
CO5	Demonstrate the principles and working of various instrumentation techniques like UV, Ultrasonic interferometer, flame photometer, cyclic voltammeter through suitable experiments.
CO6	Discuss the importance and advantages of conductometric and potentiometric titrations over volumetric titration for quantitative analysis.
CO7	Apply Beer-Lambert's law to determine unknown concentration of Fe, Cu and Ni using colorimeter by adding suitable colouring agent.
CO8	To determine strength of given KMnO 4 solution potentiometrically and to identify the formal redox potential. To explain the determination of activity coefficient, Liquid Junction Potential (LJP), Transport number by Concentration Cell method.

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	PO										PSO				
	1	2	3	4	5	6	7	8	9	10	1	2	3	4	5
CO1	3	3	3	3	2	2	3	3	3	2	3	3	3	3	3
CO2	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
CO3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
CO4	3	3	3	3	2	2	3	3	2	3	3	3	3	3	3
CO5	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
CO6	3	3	3	3	3	2	3	3	2	3	3	3	3	3	3
CO7	3	3	3	2	3	2	3	3	3	3	3	3	3	3	3
CO8	3	3	2	3	2	2	3	3	3	3	3	3	3	3	3

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. No.	LIST OF EXPERIMENTS	COs
1.	Colorimetric estimation of Copper	(CO1 &CO7)
2.	Colorimetric estimation of Iron.	(CO1 &CO7)
3.	Analysis of kidney stones by permanganometry.	(CO1&CO4)
4.	Comparison of analytical results using t-test obtained by two different volumetric methods A (Permanganometry) and B (Dichrometry) in the estimation of Fe^{2+} sample solution.	(CO2 & CO3)
5.	Comparison of analytical results using t-test, obtained with the same method on samples (soft drink A & B) to measure the percentage analyte (Sodium and Potassium) using flame photometry.	(CO2, CO3 & CO4)
6.	Determination of adsorption efficiency of metal ion (iron) using activated charcoal and Perform a Q-test on the set of data by varying time and amount of adsorbent used	(CO2 & CO3)

7.	Spectrophotometric determination of the K_a of an acid-base indicator (Methyl Orange).	(CO5)
8.	Verification of additive property of potassium permanganate and potassium dichromate using UV -visible spectrophotometer.	(CO5)
9.	To study the kinetics of saponification of Ethyl acetate by Sodium Hydroxide by conductometric titrations.	(CO6)
10.	To determine the strength of given $KMnO_4$ solution potentiometrically by redox titration (Oxalic acid or Ferrous Ammonium Sulphate) and to identify the formal redox potential in the above titration.	(CO6)
11.	Determination of activity coefficient, Liquid Junction Potential (LJP), Transport number by Concentration Cell method	(CO8)
12.	Determination of half wave potentials for Cu^{2+}, Zn^{2+}, Mn^{2+} in ammonia buffer cyclic voltammetrically.	(CO5)
13.	Determination of the velocity of ultrasonic waves in a non-electrolytic liquid by Ultrasonic Interferometry.	(CO5)

REFERENCE BOOKS:

1. D. A. Skoog, 1985, Principles of Instrumental Methods of Analysis, III Ed. Saunders College Pubs.
2. Willard Merrit, Dean and Settle. 1986 Instrumental Methods of Analysis, VI Ed. CBS Pubs.
3. A. I. Vogel, 1976. Text Book of Qualitative Inorganic Analysis III Ed. ELBS.
4. D. A. Skoog and D. M. West, 1982 Fundamental of Analytical Chemistry, IV Ed. Old Reinhord& Winston Pubs.

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**MODEL**	**ESE**
Marks (out of 50)	**60**	**60**
Remember		
Understand		
Apply	30	30
Analyze	30	30
Evaluate		
Create		

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	
Understand	
Apply	50
Analyse	50
Evaluate	
Create	

SCHEME FOR II YEAR M.Sc CHEMISTRY (2020-2021 BATCH)

SEMESTER-III								
III	Core IX	Organic Chemistry-III	6	3	40	60	100	4
	Core X	Inorganic Chemistry-III	6	3	40	60	100	4
	Core XI	Physical Chemistry-III	6	3	40	60	100	4
	Soft Skill III	-	--	3	40	60	100	2
		Internship (not less than 4 weeks)	-	-	-	-	-	2
SEMESTER-IV								
IV	Core XII	Organic Chemistry-IV	6	3	40	60	100	4
	Core XIII	Inorganic Chemistry-IV	6	3	40	60	100	4
	Core XIV	Physical Chemistry-IV	6	3	40	60	100	4
	Core XV	Physical Chemistry Practical II*	5	6	40	60	100	4
	Elective II	Organic Chemistry Practical II* **OR** Research Methodology	7	6	40	60	100	3
	Elective III	Inorganic Chemistry Practical II* **OR** Modern Instrumental Techniques	5	6	40	60	100	3
	Soft Skill IV	-		3	40	60	100	2
	Advanced Course	Analytical Chemistry Practical-II*	5	6	40	60	100	3
		Group Project / Review*	-	6	40	60	100	3

SYLLABUS FOR THIRD SEMESTER

COURSE TITLE: CORE IX - ORGANIC CHEMISTRY III

Course Code	**: 1923312**	**Credits**	**: 04**
L:T:P:S	**: 4:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

This course will expose students, the techniques involved in the structural determination of organic molecules using UV, IR, NMR Spectroscopy and Mass spectrometry as tools. In addition, aromaticity, organic photochemistry, pericyclic reaction, the synthesis of Anthocyanins, Flavones, Isoflavanones, Carotenoids and Steroids will be introduced in detail.

COURSE OUTCOMES: At the end of the Course, the Student will be able to:

CO1	They can apply woodward Ficher rule in solving organic structures. They can determine the functional groups & predict the structure of molecule using UV, IR & mass data. They can analyse & predict the geometry of biomolecules by applying ORD, CD, GS-MS.- They can apply the concept of ORD &CD in solving the geometry of cis & trans 10 methyl decalone. They can analyse biomolecules using GC-MS.
CO2	They can predict the structure of organic compounds using ^{1}H-NMR/ ^{13}C/UV/ &Mass data. By analysing the spectra, they can also able predict the structure & Stereochemistry of a simple/ complicated molecule..By using data, they can compare the geometry of a molecule.- They can characterize molecules having different functional group using mass spectroscopy .They can able to differentiate enantiomers & diastereoisomers. They can predict various types of carbon (Quartenary) using ^{13}C- NMR spectroscopy.
CO3	By applying Huckels & Craigs rule they can able to classify/ differentiate benzenoid & non-benzenoid compounds. They can predict the product under thermal /photochemical conditions.
CO4	They are able to classify the types of pericyclic reactions.They can predict the product with possible geometry & they can conclude wheather a particular type of reaction is taking place under thermal or photochemical conditions.
CO5	They can draw the structure of some important alkaloids & steroids.They can outline the synthesis of anthocyanins, flavones, isoflavnonones, carotenoids & steroids. They can examine the structure of cholesterol by chemical degradation.

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	PO										PSO				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
CO2	3	3	3	3	3	3	3	3	3	3	3	3	3	3	2
CO3	3	3	3	3	2	2	2	3	1	3	3	3	2	3	2
CO4	3	3	3	3	3	3	2	3	2	3	3	3	2	3	2
CO5	3	3	3	3	2	3	2	3	2	3	3	3	2	3	2

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	CONTENTS OF MODULE	Hrs	COs
1	**PHYSICAL METHODS FOR THE STRUCTURAL DETERMINATION OF ORGANIC COMPOUNDS : UV-IR AND MASS SPECTROMETRY, ORD, CD, AXIAL HALOKETONE RULE AND OCTANT RULE** 1.1 Organic structure determination. Principles, applications of UV-Visible spectroscopy Woodward Fischer Rule-(Derivation of Beer- lambart’s law is not required) - IR spectroscopy quantitative applications and organic structure determination. 1.2 Mass spectrometry-Instrumentation- nitrogen rule- odd and even electron rule- fundamentals- molecular ion peak, base peak, isotopic peak and meta stable ions- Mass fragmentation of functional groups- aliphatic alkanes and hydrocarbons, alcohol, phenol, carbonyl compounds- carboxylic acid, esters - Mclafferty rearrangement- amines, nitro compounds - Retro Diel's Alder reaction in Mass Spectrometry- Hydrogen transfer reaction- Tandem Mass Spectrometry – GC-MS - Analysis of Biomolecules.	**20**	**CO1**

	1.3 Optical rotatory dispersion and Cotton effect – applications-plain curves -specific rotation Vs wavelength, Molecular rotation Vs Wavelength-Non plain curves-applications-Location of methyl group at C2 or C4 in 3-cholestanone,ring size , conformational changes in menthone and degree of ketal formation. Application of ORD and CD to stereochemistry of cyclohexanone. 1.4 Axial haloketo rule and octant rule. Problem solving approach. (Applicable to 3methylcyclohexanones and cis and trans-10-methyl-2-decalone).		
2	**NMR SPECTROSCOPY (^{1}H AND ^{13}C)** 2.1 1H Nuclear Magnetic resonance spectroscopy - Chemical shift, spin-spin coupling - geminal, vicinal, long-range-1J, 2J, 3J, 4J and 5J coupling in NMR, Spin systems: Two interacting nuclei: A2, AB, AX, AA’BB’, dd, pair of doublet, AB quartet , and higher- Pople nomenclature- coupling constants, NMR and symmetry, second order effects in coupled systems, virtual coupling and shift reagents. Factors affecting coupling constant: cis, trans, gem, ortho, meta, para coupling – exchange with deuterium. 2.2 Applications to organic structure determination. FT-NMR, NOE studies, 2D NMR (COSY, HOMOCOR, HETCOR) and stereochemistry – Differentiating enantiomers and diastereomers. 2.3 ^{13}C NMR spectroscopy– Sensitivity, natural abundance, sample requirement, PFT, proton noise or broadband decoupling, Decoupling technique: SFORD and Off Resonance decoupled spectrum identification of various types of carbon using ^{13}C NMR. Quaternary carbons, chemical shifts, spin-spin coupling. Homo nuclear and heteronuclear coupling. 2.4 Applications and examples, conjoint problems (solving the structure of a compound using UV, IR, NMR spectroscopy and MASS spectrometry)	**18**	**CO2**
3	**AROMATICITY AND ORGANIC PHOTOCHEMISTRY** 3.1 Aromaticity of benzenoid, heterocyclic and non-benzenoid compounds- Huckel’s ruleAromatic systems with pi electron numbers other than six, non-aromatic and anti-aromatic systems -	**16**	**CO3**

	systems with more than 10 pi electrons – Annulenes up to C18, fulvenes, fulvalenes and azulenes – craig's rule (preparation, physical and chemical properties of all these compounds is not expected). 3.2 Photochemistry of ketones, Norrish Type I and II, photo reduction, photo addition of alpha, beta unsaturated ketones, photo cycloaddition, photo oxidation , Paterno - Buchi reaction, Di–pi methane rearrangement (bicyclic systems not required) - Barton reaction, photo- Fries reaction.		
4	**PERICYCLIC REACTIONS** 4.1 Pericyclic reaction – classification (Electrocyclic, Cycloaddition, Sigmatropic, cheletropic reactions - one example each) - Orbital symmetry-Woodword Hoffman rules. 4.2 Electrocyclic reactions -FMO and correlation diagram – Interconversion of butadiene – cyclobutene- hexatriene to cyclohexadiene. 4.3 Cycloaddition FMO and correlation diagram –(2s + 2s), (4s + 2s) –Diels alder reaction 4.4 Sigmatropic reactions- FMO method only – (1,3),(1,5) , (1,7) and (3,3) sigmatropic rearrangements – oxy cope, aza cope and Claisen rearrangements. Structure of bulvalene - fluxional molecule.	**18**	**CO4**
5	**ANTHOCYANINS, FLAVONES, ISOFLAVANONES, CAROTENOIDS AND STEROIDS** 5.1 Anthocyanins-Robinson synthesis of Cyanin (Properties and reactions not required). Flavones – general method of synthesis - Reaction with KOH- Quercetin- Robinson Method - Baker Venkatraman and Robinson syntheses. Isoflavones- Reaction with KOH -daidzein only-Spath and Baker Ollis synthesis- Carotenoids –Weedon et al synthesis of Lycopene. 5.2 Elucidation of structure of cholesterol (by chemical degradation). Conversion of cholestrol to progestrone, esterone and testosterone.	**18**	**CO5**

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ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**CIA I**	**CIA II**	**CIA III**	**ESE**
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

COURSE TITLE: CORE PAPER X - INORGANIC CHEMISTRY – III

Course Code	**: 1923313**	**Credits**	**: 04**
L:T:P:S	**: 4:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

This course will expose students, the basic and necessary techniques involved in the structural determination of inorganic and organic molecules along with their bonding characteristics using several spectroscopic domains like UV, IR, NMR, NQR, ESR and Mossbauer Spectroscopy. In addition the concept of determination of ground and excited state term symbols for dn systems is imparted to the students and the concept of correlation diagrams with electronic spectroscopy pertaining to inorganic complexes with selection rules are provided in depth. A detailed study on the stability of the inorganic complexes based on the nature of metal and ligand is also provided.

COURSE OUTCOMES: At the end of the Course, the Student will be able to:

CO1	Students will be able to explain the selection rules, predict and identify the IR stretching frequencies of some important functional groups in complexes and bonding in metal carbonyls.
CO2	Students will able to explain the principle and applications of NQR spectroscopy
CO3	Students will be able to predict and identify the ^{19}F, ^{31}P, and ^{15}N NMR spectra of various compounds. Students will use the principle of EPR spectroscopy to calculate or predict the EPR signals of both organic and inorganic compounds.
CO4	Students will use the principle of MÖssbauer spectroscopy to analyse the MÖssbauer spectra of Fe and Sn complexes.
CO5	Students will explain the selection rules for electronic spectroscopy; predict the term symbols, analyse the Orgel and T.S. diagrams.
CO6	Students will able to explain the stability constant, factors affecting stability constant, and methods of determining them.
CO7	Students will use the HSAB concept, theoretical basis of hardness and softness and explain the macrocyclic ligands.

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	PO										PSO				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	3	3	2	2	1	3	3	3	3	2	3	2	3
CO2	3	3	3	2	3	2	1	2	2	2	3	3	2	3	3
CO3	3	3	3	3	2	2	2	2	2	3	3	2	3	3	3
CO4	3	3	3	2	3	2	2	2	2	3	3	2	3	2	3
CO5	3	3	3	3	2	3	2	2	3	3	3	3	2	3	3
CO6	3	3	3	3	3	2	3	3	2	3	3	2	3	2	3
CO7	3	3	3	3	2	3	2	3	3	2	3	2	2	3	3

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. No.	CONTENTS OF MODULE	Hrs	COs
1	**SPECTROSCOPY-I** 1.1 **Infra Red Spectroscopy** 1.1.1 Selection rule-Stretching frequencies of some important functional groups. 1.1.2 Study of hydrogen bonding, effect of coordination on the stretching frequency- carboxylic acids, amides, esters, sulphato and aqua complexes-bonding in carbonyls. 1.2 **Nuclear Quadrupole Resonance Spectroscopy** 1.2.1. Quadrupole nuclei-quadrupole moment-electric field gradient (EFG): symmetrical and non-symmetrical field gradients-asymmetry parameters η- Quadrupole energy states and their interaction with the electromagnetic radiation- NMR vs NQR. 1.2.2. NQR transition energy for the axially symmetric systems (I = 3/2, 5/2, 7/2 and 1) and NQR transition energy for the non-axial	15	**CO1, CO2**

	symmetric systems (I = 3/2 and 1)- splitting by magnetic field (Zeeman effect)- conditions to observe the NQR signals- Instrumentation. Applications of NQR spectroscopy-structural determination-group 13 halides- MX_3 (M= Al; X= Cl) – BrCN, PCl_5, $SiCl_4$, - hybridization scheme- H_2S.		
2	**SPECTROSCOPY-II** 2.1 **Nuclear Magnetic Resonance Spectroscopy** ^{19}F, ^{31}P, and ^{15}N NMR spectra- introduction- structural problems of the compounds like SF_4, PF_5, BrF_5, HPF_2, H_3PO_4, H_3PO_3, H_3PO_2, P_4S_3. Isomers of Rh $(PPh_3)_3Cl_3$, [Pt $X_2(PR_3)_2$], $P_3N_3Cl_4F_2$, $P_4N_4Cl_6(NHC_6H_5)_2$, $P_3N_3(C_6H_5)_3F_3$, R_2PF_3. 2.2 **Electron Spin Resonance Spectroscopy** Introduction- information gained from EPR – *‘g’* and *‘A’* parameters- line width-presentation of EPR spectra and use of standard- *Mc-Connel equation*-Kramer's rule of degeneracy-energy level splitting in zero magnetic field-EPR spectra of transition metal ion complexes like bis(salicylaldimine) copper (II), $Co_3(CO)_9Se$, $[(NH_3)_5Co\text{-}O_2\text{-}Co(NH_3)_5]^{5+}$and Mn^{2+} complexes-representative spectra of different d^n systems- evaluation of spin-orbit coupling.	**25**	**CO3**
3	**SPECTROSCOPY-III** **MÖssbauer spectroscopy** 3.1.1 Principle-recoil energy- Doppler shift –natural width- MÖssbauer effect-Instrumentation- isomer shift or chemical shift-quadrupole splitting-Zeeman splitting (magnetic hyperfine splitting). 3.1.2 Application of Mossbauer spectroscopy in the study of iron complexes-Fe $(CO)_5$, $Fe_2(CO)_9$, $Fe_3(CO)_{12}$, spin free and spin paired Fe complexes - $K_4[Fe(CN)_6]$, $K_3[Fe(CN)_6$, $FeCl_3$, $FeSO_4.7H_2O$, $Fe[Fe(CN)_6]$ (Berlin green), sodium nitroprusside, $[Fe (NO) (H_2O)_5]^{2+}$. 3.1.3 Application of Mossbauer spectroscopy in the study of tin complexes- Oxidation states of tin in its different compounds-order of isomer shifts in R_2SnX_2 and R_3SnX-*cis* and *trans* R_2SnX_4 compounds.	**25**	**CO4, CO5**

	3.1 **Introduction to Electronic Spectroscopy** 3.2.1 Origin and different regions of electronic spectra-electron transition in metal complexes-d-d and charge transfer spectra (L-M, M-L, inter ligand, M-M transitions). L-S coupling, spectroscopic states, rules for the determination of spectroscopic states according to L-S coupling scheme. 3.2.2 Term symbols, Term states for d^n – ions (ground state for all possible d^1, d^2 and d^3), hole formulation, microstates, calculation of number of microstates-selection rules for d-d transitions. 3.2.3 Orgel correlation diagrams for octahedral and tetrahedral complexes - Mn^{2+} high spin complexes - limitations of Orgel energy diagrams. Sugano - Tanabe diagrams.		
4	**STABILITY OF COORDINATION COMPLEXES-I:** 4.1 Stability of complexes: Thermodynamic Stability – Stepwise and Overall Stability Constants and their relationships. 4.2 Factors affecting the stability of the complexes- statistical factor-electronic structure of the metal ions: charge on the central metal ion, size of the metal ion, electronegativity of the metal ion-nature of the ligand: size and charge of the ligands, basic character, chelate effect, number and size of the chelate rings, steric effect, macrocyclic effect. 4.3 Determination of stability constants by Spectrophotometric, Polarographic and Potentiometric methods.	**10**	**CO6**
5	**STABILITY OF COORDINATION COMPLEXES-I** 5.1. HSAB- Irving-Williams series of stability- classification of acids and bases as hard or soft- characteristic features of those acids and bases- - applications of HSAB principle- stability of the complexes having same ligands- stability of the complexes having different ligands, stability of the complexes having same and different ligands-prediction of chemical reactions-prediction of nature of bonding in complexes formed by ambidentate ligands-occurrence of minerals-poisoning of metal catalyst- rates of chemical reactions-limitations of HSAB principle-symbiosis.	**15**	**CO7**

	5.2. Theoretical basis of hardness and softness –ionic and covalent bond theory-pi bonding theory-Pitzer’s theory-relation of acid base strength with hardness and softness- relation of electronegativity with hardness and softness. **5.3.** Macrocyclic ligands- types, Schiff bases, template effect, Crown ethers, Cryptands.		

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ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**CIA I**	**CIA II**	**CIA III**	**ESE**
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

COURSE TITLE: CORE XI - PHYSICAL CHEMISTRY III

Course Code	**: 1923314**	**Credits**	**: 04**
L:T:P:S	**: 4:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVE

The objective of the course is to make the students to apply the concepts of quantum chemistry to chemical bonding, quantify the non-ideal nature of the electrolytes, apply the concepts of electrode kinetics for the better choice of the electrodes, prevent corrosion, develop fuel cells, determine the structure of the compounds using spectroscopy such as microwave, IR, Raman and NMR spectroscopy.

COURSE OUTCOME: At the end of the Course, the Student will be able to:

CO1	Apply LCAO-MO theory to diatomic and polyatomic molecules
CO2	Apply Huckle-Molecular orbital theory to molecules such as ethylene, butadiene, cyclobutadiene and benzene
CO3	Explain various models of the double layer and compare them to find the best model which is closure in approximation to the real structure around the electrode.
CO4	Apply the theory of activity coefficient to electrolytic solutions for practical situations
CO5	Use the theories of electrode kinetics to calculate overpotential which finds wider applications in the construction of batteries, fuel cells, electrolysis, prevention of corrosion and electroanalytical techniques such as voltammetry.
CO6	Explain the concepts of Microwave, infrared and electronic spectroscopy to determine microscopic parameters such as energy, bond length etc.
CO7	Explain the principles of nuclear resonance spectroscopy for the following magnetically active nuclei viz. ^{1}H ,^{13}C, ^{19}F, ^{31}P use this for the structural elucidation of simple molecules.

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	PO										PSO				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	3	3	1	1	1	2	1	3	3	2	3	2	3
CO2	3	3	3	3	2	2	1	2	1	3	2	3	2	2	3
CO3	3	3	3	3	1	3	1	2	2	3	2	2	3	2	2
CO4	3	3	3	3	2	1	1	2	3	3	3	3	2	3	2
CO5	3	3	3	3	1	3	1	2	2	3	3	2	3	2	3
CO6	3	3	3	3	1	2	1	2	1	3	2	2	3	2	2
CO7	3	3	3	3	2	2	1	3	3	3	2	3	2	2	3

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	CONTENTS OF MODULE	Hrs	COs
1	**CHEMICAL BONDING** 1.1 Born-Oppenheimer approximation- valence bond theory for Hydrogen molecule 1.2 LCAO-MO theory for Hydrogen molecular ion, di and poly atomic molecules-Molecular term symbols 1.3 Concept of hybridization–Hybrid orbital wave functions for sp, sp2 and sp3 hybridization 1.4 Huckel theory for conjugated molecules (ethylene, butadiene, cyclobutadiene and benzene)	**18**	**CO1, CO2**
2	**ELECTROCHEMISTRY-I** 2.1 Electrode-electrolyte interface: Electrical double layer - Electrocapillary phenomena - Lippmann equation	**18**	**CO3, CO4**

	2.2 Structure of double layer: Helmholtz -Perrin, Guoy- Chapmann and Stern models of electrical double layer. Zeta potential and potential at zero charge. 2.3 Mean ionic activity and mean ionic activity coefficient-concept of ionic strength, Debye Huckel theory of strong electrolytes-activity coefficient of strong electrolytes determination of activity coefficient. 2.4 Debye Huckel limiting law at appreciable concentration of electrolytes - Debye Huckel Bronsted equation-qualitative and quantitative verification.		
3	**ELECTRO CHEMISTRY –II** 3.1 Mechanism of electrode reaction - polarization and overpotential, activation polarization -Butler-Volmer equation for one step and multistep electron transfer reactions-significance of exchange current density- symmetry factor-transfer coefficient 3.2 Mechanism of hydrogen and oxygen evolution reactions. 3.3 Concentration polarization- principle (only) of polarography and cyclic voltammetry. 3.4 Corrosion and passivation of metals: Thermodynamics of corrosion-Pourbaix diagram, kinetics of corrosion- mixed potential theory and Evans diagram 3.5 Corrosion prevention: corrosion inhibition, Cathodic protection and passivation of metals 3.6 Fuel cells: Comparison of fuel cell with heat engine, low temperature, high temperature intermediate temperature fuel cells-acid fuel cells, base fuel cells, polymer electrolyte membrane fuel cells, molten carbonate fuel cells, solid oxide fuel cells (introductory aspects and applications)	**18**	**CO5**
4	**SPECTROSCOPY I** 4.1 Interaction of matter with radiation-Einstein's theory of transition probability. 4.2 Rotational spectroscopy of diatomic and polyatomic molecules: rigid rotor, non-rigid rotor models.	**18**	**CO6**

	4.3 Vibrational spectroscopy of diatomic and polyatomic molecules: Harmonic oscillator, effect of anharmonicity- Vibrational spectra of polyatomic molecules: Vibrational frequencies, group frequencies, vibrational coupling-overtones, combination and difference bands-Fermi resonance. Vibrational rotational lines-PQR branches 4.4 Raman Spectra: Stokes and antistokes lines- Rotational Raman spectra and Vibrational Raman spectra, OPQRS branches - Polarizability (Elementary ideas). 4.5 Electronic spectra: Molecular term symbols, Hunds rules, selection rules and electronic spectra of diatomic molecules,O2,CN-, CO and I2 4.6 Electronic spectra of polyatomic molecules: selection rules, types of transition in saturated and unsaturated hydrocarbons & formaldehyde, effect of conjugation, and solvent effects		
5	**SPECTROSCOPY II** 5.1. Resonance spectroscopy: Zeeman effect, equation of motion of spin in magnetic fields, Larmar processional frequency, gyromagnetic ratio. 5.2. Relaxation times, chemical shift-spin-spin coupling 5.3. NMR of simple AX and AMX type molecules 5.4. ^{1}H ,^{13}C, ^{19}F, ^{31}P NMR spectra, a brief qualitative discussion of Fourier transform spectroscopy.	**18**	**CO7**

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17. N. Levine, Quantum Chemistry, 6th edition.
18. Quantum Chemistry, Second Edition, Donald A. McQuarrie
19. Physical Chemistry : Robert G. Mortimer
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ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**CIA I**	**CIA II**	**CIA III**	**ESE**
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

SYLLABUS FOR FOURTH SEMESTER

COURSE TITLE: CORE XII – ORGANIC CHEMISTRY – IV

Course Code	**: 1923415**	**Credits**	**: 04**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

On taking this course, the student will be able to explain the importance of bio-organic chemistry in DNA and RNA Synthesis, demonstrate Alkaloids and Terpenoids chemistry and illustrate proteins and vitamin synthesis. In addition, the student can analyze the synthetic application of various organic reagents, protection and deprotection of functional . The student can examine the synthetic importance of organo metallic reagents using naming reactions and can create and evaluate retro synthesis and its synthetic application.

Course Outcomes: At the end of the Course, the Student will be able to:

CO1	Demonstrate and evaluate the importance and application of biomolecules like DNA, RNA and processes like transcription and translation and the synthetic methodologies for purine and pyrimidine synthesis (K4)
CO2	Develop knowledge about various synthetic routes to synthesize peptides, vitamins and biosynthesis of cholesterol (K3)
CO3	Generate ideas about alkaloid and terpenoids chemistry. (K3)
CO4	Predict and propose the synthetic route of a target molecule using disconnection approach. (K5)
CO5	Design to evaluate the modalities for the protection and deprotection of functional groups, and the usage of various reagents in organic synthesis.(K5)

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	PO										PSO				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	3	3	3	3	2	2	2	3	3	3	3	3	2
CO2	3	3	3	3	3	3	2	2	2	3	3	3	3	3	2
CO3	3	3	2	3	2	3	2	2	3	3	3	3	3	3	2
CO4	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
CO5	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	CONTENTS OF MODULE	Hrs	COs
1	**BIO-ORGANIC CHEMISTRY** 1.1 Pyrimidines–(1,3-diazines)- hybridisation, basicity, orientation in nucleophilic substitution –preparation of Purines and pyrimidines from barbituric acid and urea- preparation of cytocine from malondialdehyde and Wheeler and Liddle method 1.2 Purines-tautomerism in 2,4 dichloropyrimidine- thiamine – preparation from urea and α –cyanoester- uracil –preparation by Davidson method and adenine and guanine –Preparation of adenine by Fischer and Brederick method –Guanine – preparation by Fischer and Traub method 1.3 Structure and functions of nucleic acids- Nucleoside and nucleotide - Nucleo bases and hydrogen bonding - Chargof rule- Replication of DNA –Transcription and Translation process- Genetic code. Types and Structure of RNA –biological role of DNA and RNA-Protein synthesis and Deciphering of Genetic code.	**18**	**CO1**

2	**PROTEINS AND VITAMINS** 2.1 Peptides and their synthesis - Synthesis of tetrapeptide-general methods - Merrified synthesis of tripeptide-using Glycine, Alanine, Phenyl alanine, aspartic acid, Lysine, Cysteine, Glutamic acid and Arginine. 2.2 Vitamins: Structure and chemical synthesis of Vitamin, A_1- Weeden et.al via Reformatsky pathway, Vitamin A_2- Isler et. al method, B_2- Tishler et.al, B6-Harris and Folker et.al, Vitamin D- Lythgoe et. al. 2.3 Biosynthesis of Cholesterol synthesis of mevalolate from acetate, conversion of mevalonate from isoprene, condensation of isoprene to squalene, conversion of squalene to cholesterol- Biosynthesis of bile acids - fatty acids.	**18**	**CO2**
3	**ALKALOIDS AND TERPENOIDS** 3.1 Synthesis of cocaine -Conversion of 2, 6 dihydroxy naphthalene to bridged lactam stage of morphine –conversion of bridged lactam to codeine/morphine – conversion of parabenzoquinone to bromo keto lactone stage of reserpine-conversion of bromoketo lactone to reserpine (Total synthesis of morphine and reserpine is not required). 3.2 Terpene chemistry- limonene, Menthol, camphor, and α-pinene – Chemical synthesis.	**18**	**CO3**
4	**MODERN SYNTHETIC METHODOLOGY AND NAMED REACTIONS IN ORGANOMETALLIC CHEMISTRY** 4.1 Basic principles of disconnection approach to organic synthesis- synthon and synthetic equivalents. 4.2 Retrosynthesis of 3-Methyl-1-pentane, Methyl-3-phenyl butanoate, Aspirin, cis-1-isopropyl-2-benzyl ethylene, Geraniol, 1-phenyl-1-pentane dione, cyclopenta1,2-dione, 5,5- dimethylcyclohexane-1,3-dione and 2,6-dibromoaniline. 4.3 Ficini et al., synthesis analysis of Juvabione, Corey et al., synthesis of Longifolene, cubane and Z jasmine 4.4 Barton-McCombie reaction. Buchwald-Hartwig cross coupling reaction. Heck reaction Sonogashira coupling, Julia-Lythgoe	18	**CO4**

	Olefination, Chan-Lam coupling, Elington reaction, Negishi coupling, Kumada and Suzuki coupling (with mechanism) 4.5 Glaser, Hay, Cladiot-Chodkiewicz, Sharpless reaction - aymmetric amino hydroxylation and asymmetric dihydroxylation, Stille, Hiyama, Hiyama-Denmark,. Fukuyama reduction- Corey-Bakshi-Shibata reduction. Jacobsen-Katsuki, Prilezhaev-Sharpless, Kullinkovich, Kullinkovich-de meijere and Kullinkovich-Szymoniak reactions. Luche reduction. Mc Murry coupling (Without mechanism) **Assignment topics: Study of Anti microbial and Anti bacterial activity of Organo metallic compounds.**		
5	**PROTECTION OF FUNCTIONAL GROUPS, REAGENTS AND ITS APPLICATIONS IN ORGANIC SYNTHESIS AND FREE RADICAL REACTIONS** 5.1. Protection and deprotection of functional groups (R-OH, RCHO, R-CO-R, R-NH_2 and R- COOH). 5.2. Uses of the following reagents: 9BBN, Trimethylsilyl chloride and iodide, 1,3-dithiane (Umpolung), diisobutylaluminimumhydride (DIBAL), DMSO, PCC, DCC, DMAP, DEAD, TEMPO, LDA, n-butyl lithium, Dess-Martin reagent, Catechol Boranes, Enamines- alkylations and acylations. Application of synthetic methodology for the synthesis of target molecules - through 1,3 dithianyl derivative. 5.3. Long lived and short lived free radicals, sources - methods of generation and detection of free radicals by Paneath and ESR techniques. Decomposition of diazocompounds, phenol-coupling - Sandmeyer reaction – Gomberg-Bachmann reaction, Pschorr reaction, Ulmann reaction, Hunsdicker reaction.	**18**	**CO5**

TEXTBOOKS:

1. Stuart Warren, Paul Wyatt, Organic Synthesis: The disconnection approach,2nd edition , Wiley and sons , 2008.
2. Carey F.A. and Sundberg, R.J., Advanced Organic Chemistry, 4th Edition, Plenum Press, New York, 1990.
3. Finar, I.L. Organic Chemistry – Vol.II, 5th edition, ELBS Publication 1986.
4. March J. and Smith M.B., March's Advanced Organic Chemistry: Reactions, Mechanisms and structure, 6th edition, Wiley, 2007
5. House H.O., Modern Synthetic Reactions, The Benjamin Cummings Publishing Company, London, 1972.
6. Gupta B.D., Elias A.J. Basic oraganometallic chemistry: Concepts synthesis and applications of transition metals, Universities Press, 2010.
7. Jonathan Clayden, Nick Greeves & Stuart Warren, Organic Chemistry, Second Edition, Oxford University press, 2012.

REFERENCE BOOKS:

1. Stuart Warren, Paul Wyatt, Organic Synthesis: Strategy and control, First edition, Wiley and sons , 2007.
2. Bansal, R.K, Heterocyclic chemistry, 5th ed., New age International pvt ltd publishers, 2015.
3. Sainsury, M., Heterocyclic chemistry, Wiley, 2014.
4. Eicher, T., Hauptmann, S., Speicher, A., The chemistry of heterocycles: Structure, reactions, synthesis and applications 3rd ed., John wiley& sons, 2013.
5. Pozharskii, A.F., Soldatenkov, A. and Katritzky, A.R., Heterocycles in life and society, Wiley, 2011.
6. Parashar, R.K, Heterocyclic chemistry, ANE books, 2010.
7. Ahluwalia, V.K., Terpenoids, ANE books, 2009.
8. Talapatra S.K. and Talapatra B., Chemistry of natural products: Stereochemistry, conformation, synthesis, biology and medicine, Springer, 2015.
9. Neil S. Issacs, Physical Organic Chemistry, ELBS Publication, 1987.
10. Nakanishi, K. Goto, T.and Ito, S., Natural products chemistry Vol. 1 and 2, Academic press, 2013.
11. Lednicer, D., Steroid chemistry at a glance, Wiley, 2011.

12. Kalsi, P.S. Texbook of Organic Chemistry, Mcmillan India Ltd., 1999.
13. Mehrotra R.C.and Singh A., Organometallic chemistry -A unified approach, New age international Ltd., New Delhi, 2009.
14. Carruthers W., Some Modern Methods of Organic Synthesis, 3rd Edition Cambridge University Press, 1993.

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3. https://courses.stu.qmul.ac.uk/NatSci/sbcs/info/home.htm%20
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7. https://courses.stu.qmul.ac.uk/NatSci/sbcs/info/webmaths.htm
8. http://webbook.nist.gov/chemistry/
9. http://www.organic-chemistry.org/
10. http://www.orgsyn.org/

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	CIA I	CIA II	CIA III	ESE
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	Weightage %
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

COURSE TITLE: CORE XIII - INORGANIC CHEMISTRY - IV

Course Code	**: 1923416**	**Credits**	**: 04**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

This course will expose students, the concept, theories and mechanism of substitution in 6 and 4 membered Octahedral and Square planar complexes respectively with respect to ligands and the isomerism arising from it. The concept of associative, dissociative mechanism and Marcus theory is provided in detail. The concept of photochemistry is introduced related to photooxidation, photoderuction, photosubstitution and photosensitization related to select Ru, Fe, Co and Cr complexes. A brief concept and role of nuclear processs, reactors and counters along with the knowledge involved in fission and fusion reactions in stars are explained in detail.

COURSE OUTCOMES: At the end of the Course, the Student will be able:

CO1	To assess the Ligand Substitution Reactions mechanism and its limitations, electron transfer reactions (K3)
CO2	To evaluate the Substitution in complexes and theories of Trans effect and its applications (K5)
CO3	To analyse various Nuclear Chemical reactions, examine various types of nuclear reactors, effect of radiation chemistry (K3, K5)
CO4	To evaluate the Photochemical reaction of metal Carbonyls and complexes (K4)

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	**PO**										**PSO**				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	2	3	2	2	3	3	2	2	2	3	3	3	3	2
CO2	3	2	2	3	2	3	3	2	2	2	3	3	3	3	2
CO3	3	2	3	3	3	3	3	3	3	3	3	3	3	3	3
CO4	3	2	3	3	3	3	3	2	3	2	3	2	3	3	3

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	CONTENTS OF MODULE	Hrs	COs
1	**COORDINATION COMPOUNDS -REACTION MECHANISMS I** 1.1 Introduction: Lability-inertness-interpretation in terms of Valence Bond theory, Crystal Field theory of Octahedral complexes-CFAE; applications and limitations of CFAE-types of ligand substitution reactions-mechanism: dissociative mechanism (D), associative mechanism (A), Interchange mechanism (I). General rate law for A, D and I. Limitations of the rate law and mechanisms of ligand substitution reactions-distinction between D, I_d, I_a pathways. 1.2 Substitution of octahedral complexes of cobalt and chromium, replacement of coordinated water, solvolytic (acid and base catalysed) reactions -anation reaction. Substitution reaction without the cleavage of M-L bond. 1.3 Electron transfer reactions; outer and inner sphere processes; atom transfer reaction, complementary and non-complementary reactions. 1.4 Formation and rearrangement of precursor complexes, bridging ligand, role of bridging ligand with ISET reaction- tunneling transfer -multiple bridging in the activated complex in ISET successor complexes, Marcus theory.	**30**	**CO1**
2	**COORDINATION COMPOUNDS - REACTION MECHANISMS II** 2.1 Substitution in square planar complexes, reactivity of platinum complexes, influences of entering, leaving and other groups- Swain Schott equation. 2.2 Trans influence- Trans effect- trans effect series-theories of trans effect (polarization theory, pi bonding theory, sigma bonding theory and Cardwell's electronegativity theory) and applications of trans effect. 2.3 Synthesis of Pt[ABCD] type complexes and methods to differentiate the isomers-Kurnakov test.	**10**	**CO2**
3	**NUCLEAR CHEMISTRY-I** 3.1 Nuclear properties: nuclear charge, nuclear radius, even-odd nature of nucleus (Oddo-Harkin's rule)-nucleon pairing –nuclear stability and positron emission-nuclear spin and moments, origin of nuclear forces-Yukawa's theory. 3.2 Modes of radioactive decay: orbital electron capture; nuclear isomerism, internal conversion.	**15**	**CO3**

	3.3 Nuclear reaction: Types-projectile capture reaction-projectile capture particle emission reaction-spallation reaction- nuclear fission and fusion reactions as energy sources- photonuclear reactions- thermonuclear reactions-reaction cross section, Q-value, threshold energy, compound nucleus theory: high energy nuclear reactions,		
4	**NUCLEAR CHEMISTRY-II** 4.1 Nuclear reactors: Types-Power reactor-principle of operation-components of a power reactor-critical fuel assembly- Fast breeder reactors, particle accelerators, linear accelerators, cyclotron, synchrotron and synchrocyclotron. Units of nuclear radiation-detection and determination of activity by cloud chamber, nuclear emulsion, bubble chamber, G.M., Scintillation and Cherenkov counters. 4.2 Stellar energy: Hydrogen and carbon burning, the *e, s, r, p* and *x* process. 4.3 Radiation Chemistry-Chemical effects of radioactive decay-hot atom-epithermal reactions-applications-isomeric transition- radiolysis of water-formation of ionic products-formation of free radicals-formation of hydrated electrons-Hart and Baog’s experiment-properties of hydrated electron. Radio immunoassay (RIA).	**20**	**CO3**
5	**INORGANIC PHOTOCHEMISTRY** 5.1. Photochemical excitation-prompt and delayed reaction-photochemical reaction of metal carbonyls. Co (III) complexes, Cr (III) complexes-photolysis of $[M(CN)_8]^{3-}$ and $[M(CN)_8]^{4-}$ (M= Mo, W) in aqueous solution-oxalato complexes $[M(ox)_3]^{3-}$ (M= Fe, Mo, Co). 5.2. Photochemical reaction of Fe (II) and Fe (III) complexes-photochemical substitution process in Pt (IV). 5.3. Photochemistry of $[Ru(bpy)_3]^{2+}$ and its applications in solar energy conversion-photochemical splitting of H_2O-TiO_2 as a green photocatalyst in removing air and water pollutants. 5.4. Photochemical reactions of nitrogen	**15**	**CO4**

TEXT & REFERENCES BOOK:

1. Purcell, K.F. and Kotz, J.C., - Inorganic Chemistry, WB Saunders Co., USA (1977)
2. J.E. Huheey, 1993, Inorganic Chemistry - Principles, Structure and Reactivity; IV Edition, Harper Collins, NY.
3. M. C. Shrivers, P. W. Atkins, C H Langford, Inorganic Chemistry, OUP, 1990.
4. F. Basolo and Pearson, Mechanism of Inorganic Reactions, Wiley, New York, 1967.
5. F.A. Cotton and G. Wilkinson, 1988, Advanced Inorganic Chemistry - A Comprehensive Text, V. Edition, John Wiley & Sons.
6. Photochemistry of Inorganic coordination compounds by Balzani.
7. C.R. Choppin and J. Ryd Berg: Nuclear Chemistry - Theory and Applications, Pergamon Press.
8. B.G. Harvey, Introduction to Nuclear Physics and Chemistry Prentice Hall, 1962.
9. H.J. Arnikar, Nuclear Chemistry, Wiley Eastern Co. II Edition 1987.
10. Glasstone & Sesonske – Nuclear reactor engineering.
11. C. Kellter: Radiochemistry, Ellis Hardwood Ltd., John Wiley and Sons.
12. G.R. Chopin, Experimental Nuclear Chemistry, Prentice Hall, 1962.
13. G. Friedlander, J.W. Kennedy, and J.M. Miller, Nuclear and Radio Chemistry, John Wiley.
14. N.J.Turro. Modern Moleular Photochemistry, Benjamin, Cummings, Mento Park, California 1978
15. K.K.Rohatgi Mukherjee. Fundamentals of Photochemistry, Wiley Eastern Ltd.,
16. A.W.Adamson and P.Fleischauer Concepts of Inorganic Photochemistry, Wiley, 1975.
17. Advanced Inorganic Chemistry Vol I and II by S. P. Banerjee. Books and Allied (P) Ltd. 2003.

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**CIA I**	**CIA II**	**CIA III**	**ESE**
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

COURSE TITLE: CORE XIV - PHYSICAL CHEMISTRY – IV

Course Code	**: 1923417**	**Credits**	**: 04**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

To learn the basics of classical and quantum distribution of particles and its applications, basic and applied photochemistry principles, and introduction to material chemistry.

COURSE OUTCOMES: At the end of the Course, the Student will be able:

CO1	To enumerate on various distribution of microscopic particles and contemplate on partition function.[K1]
CO2	To articulate partition function for various thermodynamic functions, and discuss heat capacity of solids. [K3]
CO3	To compute Jablonski diagram, establish enhancement and quenching process. [K3]
CO4	To organise Photophysical, Photochemical processes and distinguish Photovoltaic, Photogalvanic cells. [K4]
CO5	To prioritize the properties of solids and persuade the solid state ionics.[K4]

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	**PO**										**PSO**				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	3	3	3	3	2	2	2	3	3	3	3	3	2
CO2	2	3	3	3	3	3	2	2	2	3	3	3	3	3	2
CO3	3	3	2	3	2	3	2	2	3	3	3	3	3	3	2
CO4	3	3	3	3	2	3	3	3	3	3	3	3	3	3	3
CO5	3	3	3	3	3	3	3	3	3	3	3	3	2	3	3

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	CONTENTS OF MODULE	Hrs	COs
1	**STATISTICAL THERMODYNAMICS-I** 1.1 Microstates and Macrostates, most probable distribution, Concept of thermodynamic probability - distribution of distinguishable and non-distinguishable particles. 1.2 Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein statistics, modes of contribution to energy. 1.3 Partition functions: Translational, Vibrational, Rotational, Electronic and Nuclear partition functions for mono, diatomic and polyatomic ideal gases.	18	CO1
2	**STATISTICAL THERMODYNAMICS-II** 2.1 Concept of Ensemble, Thermodynamic functions in terms of partition functions. 2.2 Equilibrium constant for isotope exchange and dissociation of diatomic molecules. 2.3 Heat capacity of solids (Einstein and Debye Models). 2.4 Planck's radiation law- Electrons in metals, Ortho and Para hydrogen	18	CO2
3	**PHOTOCHEMISTRY-I** 3.1 Absorption and emission of radiation-Franck-Condon Principle. 3.2 Decay of electronically excited states – Jablonski diagram- Radiative and Non radiative processes: fluorescence and phosphorescence-spin forbidden radiative transition internal conversion and intersystem crossing 3.3 Energy transfer process: Excimers and Exciplexes 3.4 Quenching: Static and Dynamic quenching-Stern Volmer analysis.	18	CO3
4	**PHOTOCHEMISTRY-II** 4.1 Quantum yield, determination of quantum yield using standard quantum yield references Actinometry. 4.2 Flourescence life time measurements- Flash photolysis using Nd-YAG Laser, time correlated single photon counting techniques, instrumentation and application 4.3 Kinetics of photophysical and photochemical reactions. 4.4 Photovoltaic and photogalvanic cells. photoelectrochemistry, Aspects of solar energy conversion.	18	CO4

5	**INTRODUCTION TO PHYSICAL ASPECTS OF MATERIALS** 5.1. Introduction - Properties of materials and some important relationships 5.2. Free electron theory of metals, Drude model- Wiedemann Franz law, Drude Sommerfeld model. 5.3. Anisotropy in crystal, Periodic potential, Electronic contribution to specific heat at constant volume-Incorporating crystal structure in model-introduction to reciprocal space, Condition for diffraction, Ewald sphere, simple cubic, FCC, BCC in reciprocal space, Wigner Seitz cell and introduction to Brillouin zones-Calculation of Allowed energy gaps and forbidden gaps, Bands -Free electron approximation, Tight binding Approximations 5.4. Addressing specific material properties using the model developed-Semiconductors, superconductors, optoelectronic properties, nanoscale materials (elementary approach).	18	CO5

REFERENCE:

1. J.Rajaram & J.C.Kuriacose,1993, Thermodynamics for students of chemistry
2. K.K. Rohatgi Mukherjee, 1978, Fundamentals of Photochemistry, Wiley Eastern Ltd.
3. N.J. Turro, 1978, Modern Molecular Photo chemistry, Benjamin, Cummings, Menlo Park, California
4. Statiscal thermodynamics by B.J. McClelland.
5. Statistical thermodynamics by Andrew Maczek
6. An Introduction to Statistical Thermodynamics (Dover Books on Physics) By Terrell L. Hill (Author).
7. Theoretical chemistry by Samuel Glasstone.
8. Thermodynamics, kinetic theory and Statiscal Thermodynamics by Sears.Salinger.
9. Bernard Valeur Molecular Fluorescence Principles and Applications.
10. Principles of Fluorescence Spectroscopy | Joseph R. Lakowicz .
11. Heat and thermodynamics and statiscal physics by Brijlal N. Subramanyam and P.S. Hemne.
12. Principles of photochemistry and photo physics by Bulzani
13. Physics of materials: Essential concepts of solid-state physics – Prathap Haridoss – IIT Madras- Wiley publishers

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**CIA I**	**CIA II**	**CIA III**	**ESE**
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

CORESE TITLE: CORE XV - PHYSICAL CHEMISTRY PRACTICALS II

Course Code	**: 1923418**	**Credits**	**: 04**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

To understand and verify the concepts and equations in physical chemistry by carrying out the following suitable experiments.

Course Outcomes: At the end of the Course, the Student will be able to:

CO 1.	To verify laws based on electrochemistry, to determine end point of various titrations, to evaluate the solubility product using conductometer.
CO 2	To determine pH, pKa , to determine end point of various titrations, to evaluate the solubility product and stability constant using Potentiometer
CO 3.	To evaluate the endpoint of poly basic acid titration using pH meter.
CO 4.	To lead students to have a comprehensive approach to structural identification of molecules from the spectral data.

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	**PO**										**PSO**				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	3	3	2	3	2	2	2	3	3	3	3	3	2
CO2	3	3	2	3	2	3	2	2	2	3	3	3	3	3	2
CO3	3	3	3	3	2	3	2	3	2	3	3	3	2	3	2
CO4	3	3	2	2	2	3	2	2	2	3	3	3	2	3	2

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. No.	CONTENTS OF MODULE	COs
1	**CONDUCTOMETRIC EXPERIMENTS** 1.1 Determination of equivalent conductance of strong electrolytes and verification of Debye- Huckel- Onsager equation. 1.2 Determination of dissociation constant of weak electrolytes using Ostwald's dilution law. 1.3 Conductometric titrations between simple and mixture of strong and weak acids and strong base. 1.4 Condutometric titration of mixture of weak acid and salt of weak acid and strong base. 1.5 Conductometric titration of weak acid against weak base. 1.6 Precipitation titrations involving a single halide and BaCl2 with MgSO4. Determination of solubility product. 1.7 Determination the degree of hydrolysis and hydrolysis constant of sodium acetate conductometrically. 1.8 Determination the concentrations of H2SO4, CH3COOH and CuSO45H2O in a mixture by conductometric. titration with sodium hydroxide 1.9 Determine Critical Micellar Concentration (CMC) of sodium lauryl sulphate [Soap soln] from the measurement of conductivities at different concentrations	**CO1**
2	**POTENTIOMETRIC EXPERIMENTS** 2.1 Determination of pH and calculation of pKa –Buffer value 2.2 Determination of solubility product of a sparingly soluble salt. 2.3 Potentiometric titrations between simple and mixture of strong and weak acids with base. 2.4 Redox titrations by emf measurements. 2.5 Precipitation titration of mixture of halides by emf measurements. 2.6 Determination of composition of complex 2.7 Potentiometric titration of poly basic acid. 2.8 Potentiometric titration of Mixture of acids vs strong base 2.9 Solubility product determination by emf measurements 2.10 Determine the stability constant of the complex ion Ag (S2O3)23- potentiometrically.	**CO2**

3	**pH TITRATIONS** 3.1 Acid-Base titration-Mixture of acids vs strong base 3.2 Polybasic acid titration	**CO3**
4	**SPECTRAL ANALYSIS-INTERPRETATION** 4.1 IR spectral data-Determination of force constant, zero point energy, application of group theory concepts. 4.2 Vibrational rotational spectral data-line spacing, bond length 4.3 Rotational spectral data- Determination of internuclear distance 4.4 Raman spectra, data-identification of stokes, anti-stokes lines, interpretation of intensity pattern, and depolarization ratio-application in identification in modes of vibration. 4.5 Interpretation of IR, Raman data-application of Mutual Exclusion principle. Electronic spectral data-application of Beer-Lambert's Law, energy calculations, type of transitions, effect of solvent on intensity pattern, application of Huckel's model on extended conjugation in the case of real system. 4.6 NMR data-identification of peaks, spin multiplicity, chemical shift, coupling constant, identification of nature of protons in NMR spectrum-identification of nature of 13C nuclei in CMR spectra. 4.7 A comprehensive approach to structural identification of molecules from the spectral data. (only for practice)	**CO4**

REFERENCES:

1. M.Sc. Physical Chemistry Practical manual-II Edited by Dr. S. Bangaru Sudarsan Alwar,; Dr. C. Srinivasan,; R. Ramesh Kumar,; V. Rajagopaln. Department of Chemistry, D. G. Vaishnav College, Arumbakkam, Chennai- 600 106.
2. Practical Physical Chemistry- Editied by Prof. B. Viswanathan, V. R. Vijayaraghavan, T. Sundravadivelu, Kamala Govidarajan, S. Vivekanandan and V. Kannapan. School of Chemistry, University of Madras, Guindy Campus.1996

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**MODEL**	**ESE**
Marks (out of 50)	**60**	**60**
Remember		
Understand		
Apply	30	30
Analyze	30	30
Evaluate		
Create		

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	
Understand	
Apply	50
Analyse	50
Evaluate	
Create	

ELECTIVE II

COURSE TITLE: ORGANIC CHEMISTRY PRACTICALS-II

Course Code	**: 1923419**	**Credits**	**: 04**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

This course comprises of three parts. The students are trained to I. Prepare organic compounds involving two stages and to determine their yield. II. To estimate organic compounds III. To extract organic compounds from natural resources.

COURSE OUTCOMES: At the end of the Course, the Student will be able to:

CO1	Structure two stage preparations of organic compounds.
CO2	Estimate the given organic compound titrimetrically
CO3	Extract simple phytochemicals from natural source and detects purity and yield.
CO4	Interpret spectra from the knowledge of spectroscopic tools.

MAPPING OF COURSE OUTCOMES TO PROGRAMME OUTCOMES & PROGRAMME SPECIFIC OUTCOMES:

CO/PO/PSO	**PO**								**PSO**				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	3	2	2	3	3	3	2	3	3	3	3
CO2	3	3	3	2	2	3	2	3	3	3	2	3	3
CO3	3	3	3	2	3	3	2	2	3	3	3	3	3
CO4	3	3	3	1	3	3	1	2	3	2	3	3	1

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. No.	**CONTENTS OF MODULE**	**COs**
1	**ORGANIC PREPARATION** **GREY SYNTHESIS** **1.** Preparation of m-Nitro benzoic acid from methyl benzoate**.** 2. Preparation of 2-phenyl indole from benzaldehyde 3. *Comparison of green and grey method (phthalimide from phthalic anhydride). 4. Preparation of Benzoin from benzaldehyde – benzil from benzoin. Benzilic acid from benzaldehyde. 5. Benzophenone oxime from benzophenone- benzophenone oxime to benzanilide 6. *Preparation of Isatin via Indigo from Anthranilic acid. **GREEN SYNTHESIS** 7. Acetylation of primary amine using zinc dust 8. Nitration of phenol using calcium nitrate 9. Radical coupling reaction – preparation of 1,1 – bis -2- naphthol	**CO1**
2	**ORGANIC ESTIMATION** 1. Estimation of aniline by bromination (Bromate- Bromide) method 2. Estimation of phenol by bromination (Bromate- Bromide) method 3. Estimation of glucose (Bertrand's Method) 4. Estimation of glycine by Sorensen's Formol method 5. Estimation of formaldehyde (formalin) 6. Estimation of acetic acid in commercial vinegar. **7.** Estimation of Vitamin C (Reduced)	**CO2**
3	**ANY TWO EXERCISES IN THE EXTRACTION OF NATURAL PRODUCTS:** 1. Caffeine from tea leaves 2. Lactose from milk 3. Citric acid from lemon 4. Piperine from black pepper 5. Lycopene from tomato paste	**CO3**
4	**SPECTRAL INTERPRETATION OF THE FOLLOWING ORGANIC COMPOUNDS (UV, IR, PMR AND MASS SPECTRA)** 1. 1, 3, 5-Trimethylbenzene	**CO4**

	2. Pinacolone 3. n-Propyl amine 4. p-Methoxybenzyl alcohol 5. Benzyl bromide 6. Phenyl acetone 7. 2-Methoxyethyl acetate 8. Acetone 9. Isopropyl alcohol 10. Acetaldehyde diacetate 11.2-N, N-Dimethylamino ethanol 12. Pyridine 13. 4-Picoline 14. 1, 3 dibromo-1, 1-dichloropropene 15. Cinnamaldehyde. 16. Sucrose 17. Citral	

REFERENCE

1. Arthur I. Vogel, A Text Book of Practical Organic Chemistry.
2. Spectrometric identification of organic compounds by R.M.Silverstein, G.C.Basseller and Monsil, John Wiley and sons, Newyork.
3. Spectroscopy of organic compounds by P.S.Kalsi, Wiley Eastern Ltd., Chennai.
4. Raj K. Bansal, Laboratory Manual of Organic Chemistry, Wiley Eastern Limited.
5. Mann and Saunders, Laboratory manual of Organic Chemistry

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**MODEL**	**ESE**
Marks (out of 50)	**60**	**60**
Remember		
Understand		
Apply	30	30
Analyze	30	30
Evaluate		
Create		

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	
Understand	
Apply	50
Analyse	50
Evaluate	
Create	

DISCIPLINE SPECIFIC ELECTIVE COURSE-II (DSE)

COURSE TITLE: RESEARCH METHODOLOGY (90 HOURS)

Course Code	**:**	**Credits**	**: 04**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

To learn the Scientific awareness and selection of research problem, Literature Survey, Collection of Data, Reporting and thesis writing and also Computer Applications

COURSE OUTCOMES: At the end of the Course, the Student will be able:

CO1	To enumerate on scientific awareness and selection of research problem. [K1]
CO2	To articulate thorough literature survey using various resources. [K3]
CO3	To organize the data collection process. [K3]
CO4	To organise the reports and writing the thesis. [K4]
CO5	To enumerate the computer aided applications like chem. Draw, excel , origin etc. [K4]

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	**PO**										**PSO**				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	3	3	3	3	2	2	2	3	3	3	3	3	2
CO2	2	3	3	3	3	3	2	2	2	3	3	3	3	3	2
CO3	3	3	2	3	2	3	2	2	3	3	3	3	3	3	2
CO4	3	3	3	3	2	3	3	3	3	3	3	3	3	3	3
CO5	3	3	3	3	3	3	3	3	3	3	3	3	2	3	3

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	CONTENTS OF MODULE	Hrs	COs
1	**Unit 1 Scientific awareness and selection of research problem** 1.1 General scientific awareness; Objectives of research-What makes one to do research? Research design - meaning, Need for research, Components of research design, various stages of research - selection of research problem and hypothesis. 1.2 Basic principles of experimental design-important experimental design-Basic research 1.3 Possible approaches to be adopted by a researcher; factors affecting quality of research, 1.4 Problems encountered by researchers in India	18	CO1
2	**Unit 2 Literature Survey** 2.1 Primary and secondary sources-reviews, treaties, monographs, patents, current literature search methods, abstraction of research papers, 2.2 Major secondary sources-bibliography databases, 2.3 Web as a source of information, searching the web. 2.4 Literature search using Sci-finder scholar, Scopus.	18	CO2
3	**Unit 3 Collection of Data** 3.1 Collection of primary data-observation method, interview method and survey methods, Survey Techniques and Methods – Treatment of data- t-test., Q-test, F-test, significant figures and its importance – 3.2 Sources of error in research data, tests for sound measurement-Techniques of developing measurement tools - Processing and analysis of data-Statistical methods.	18	CO3

	3.3 Measures of central tendency - measures of relationship, simple regression analysis, multiple correlation and regression		
4	**Unit 4 Reporting and thesis writing** 4.1 Structure and components of scientific papers, technical reports and thesis –planning the scientific paper-contents of scientific papers and reports-Illustrations and tables. 4.2 Plots – diagrams – structures and figures presentation - Preparation of final manuscript /thesis-mechanics of writing a research report-proof reading / correction of research manuscript, style manuals. 4.3 Bibliography referencing and foot notes etc. Issues related to copyright-reproduction of published materials-royalty - Patenting	18	CO4
5	**Unit 5 Computer Applications** 5.1 Drawing structures using Chem. Draw. 5.2 Application of Excel programme for drawing tabular columns – plots – doing simple calculations. 5.3 Online submission of research articles.	18	CO5

References

1. J.Anderson Durston and pools; THESIS AND ASSIGNMENT WRITING, New Delhi; Wiley Eastern, 1970

2. Joseph Gibald MLA HAND-BOOK FOR WRITERS OF REASEACH PAPERS 6th edition New Delhi; Affiliated East-west press, 2003

3. T.S.Wilkinson and P.L Bhandarkar, METHODOLOGY AND TECNIQUES OF SOCIAL RESEARCH, Bombay; Himalaya publishing company, 2001

4.Periannan,S.sebastian, SOCIAL RESEARCH METHODOLOGY An introduction Chennai, University of Madras; Department of Christian studies,2003

4. E.Sreedharan-A TEXT BOOK OF HISTORIOGRAPHY 500 B.C to A.D 2000, Bombay, Orient Longman, 2004

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**CIA I**	**CIA II**	**CIA III**	**ESE**
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

ELECTIVE – III
COURSE TITLE: INORGANIC CHEMISTRY PRACTICAL – II

Course Code	**: 1923420**	**Credits**	**: 04**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

I. To estimate the metal ions from the given mixture of Inorganic compounds using lab techniques.
II. To prepare various metal complexes involving Cu, Ni, Co
III. Interpretation of spectra

COURSE OUTCOMES: At the end of the Course, the Student will be able:

CO1	To estimate the metal ions in the given mixture (K5)
CO2	To prepare various complexes involving , Cu, Cr, Ni, Al (K3)
CO3	To interpret NMR, ESR, IR and MB of various compounds, complexes (K3)

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	**PO**										**PSO**				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	3	3	2	2	3	2	3	2	3	2	3	3	3
CO2	3	3	3	3	2	2	3	2	3	2	3	2	3	3	3
CO3	3	3	3	2	2	2	3	2	2	2	3	2	3	3	3

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S. NO	CONTENTS OF MODULE	COs
1	**QUANTITATIVE ANALYSIS:** 1. Mixture of iron and magnesium. 2. Mixture of iron and nickel 3. Mixture of copper and nickel 4. Mixture of copper and zinc. 5. *Mixture of Calcium and Magnesium. 6. Mixture of Iron and Copper.	CO1
2	**COMPLEX PREPARATION** 1. Potassium (trisoxalato aluminate III) trihydrate. 2. (Tris thiourea copper I) chloride 3. Potassium trisoxalato chromate (III) trihydrate 4. Sodium bisthiosulphato cuprate (I) 5. Tristhiourea copper (I) sulphate 6. Sodium hexanitrocobaltate (III) 7. Chloropentamminecobalt (III) chloride 8. Bisacetylacetanato copper (II) 9. Hexamminenickel (II) chloride	CO2
3	**SPECTRAL INTERPRETATION:** 1. List of spectra to be given for interpretation 2. ^{31}P NMR Spectra of methylphosphate. 3. ^{31}P NMR Spectra of HPF_2 4. ^{19}F NMR Spectra of ClF_3 5. ^{1}H NMR Spectra of Tris (ethylthioacetoacetanato) cobalt (III) 6. Expanded high resolution ^{1}H NMR Spectra of (N-propyl isonitrosoacetylacetoneiminato) (acetylacetoneiminato) Nickel (II) 7. ESR Spectra of the aqueous $ON(SO_3)_2^{2-}$ ion. 8. ESR Spectra of H atoms in CaF_2.	CO3

	9. ESR Spectra of $[Mn(H_2O)_6]^{2+}$ ion. 10. ESR Spectra of bis (salicyladiminato) copper (II). 11. IR Spectra of the sulphato ligand. 12. IR Spectra of nitro and nitropentaminecobalt (III) chloride. 13. IR Spectra of dimethylgyloxime ligand and its Nickel (II) complex. 14. IR Spectra of Carbonyls. 15. Mossbauer spectra of $FeSO_4.7H_2O$. 16. Mossbauer spectra of $FeCl_3$ 17. Mossbauer spectra of $[Fe(CN)_6]^{3-}$. 18. Mossbauer spectra of $[Fe(CN)_6]^{4-}$. 19. Electronic spectra of $[Co(en)_3]^{3+}$ 20. Electronic spectra of $[Cr(NH_3)_6]^{3+}$ 21. Electronic spectra of Cis and Trans $[Co(en)_2(Cl)_2]^{2+}$	

*** Not for examination**

TEXT & REFERENCE BOOKS:

1. Text book of Inorganic quantitative analysis by Vogel.
2. Principles of Instrumental Analysis: Douglas A.Skoog, 3rd Edition.
3. Physical Methods in Inorganic Chemistry: R.S.Drago. Reinhold NY. 1968.
4. R.V. Parish, NMR, NQR, EPR, and Mossbauer Spectroscopy in Inorganic Chemistry. Ellis Horwood Limited. 1990.

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**MODEL**	**ESE**
Marks (out of 50)	**60**	**60**
Remember		
Understand		
Apply	30	30
Analyze	30	30
Evaluate		
Create		

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	
Understand	
Apply	50
Analyse	50
Evaluate	
Create	

ELECTIVE PAPER III

COURSE TITLE: MODERN INSTRUMENTATION TECHNIQUES (90 Hrs)

Course Code	**:**	**Credits**	**: 04**
L:T:P:S	**: 6:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OBJECTIVES:

This course is offered for students to have exposure to the various purification techniques involved in synthesis. Students get clear knowledge in both principles and application of spectroscopy like UV-Visible, NMR, ESR, Mossbauer, Photoelectron and Mass spectrometry and also electro-analytical techniques and better understanding in magnetic properties.

Course Outcomes: At the end of the Course, the Student will be able to:

CO 1.	To enumerate on advanced purification techniques in organic and inorganic preparations. [K1]
CO 2	To prioritize both principles and application of spectroscopy like UV-Visible, NMR, ESR, Mossbauer, Photoelectron and Mass spectrometry [K3]
CO 3.	To identify different decomposition temperature of the samples and thermal stability from TGA/DTA thermogram. To determine the phase transition temperature from DSC. [K3]
CO 4.	To deduce and quantify the presence of metal ions by electro-analytical techniques. [K4]
CO 5.	To analyse the magnetic properties of compounds.[K3]

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	**PO**								**PSO**				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**1**	**2**	**3**	**4**	**5**
CO1	**3**	**3**	**3**	**3**	**2**	**3**	**2**	**2**	**3**	**3**	**3**	**3**	**2**
CO2	**3**	**3**	**2**	**3**	**2**	**3**	**2**	**2**	**3**	**3**	**3**	**3**	**2**
CO3	**3**	**3**	**3**	**3**	**2**	**3**	**2**	**3**	**3**	**3**	**2**	**3**	**2**
CO4	**3**	**3**	**3**	**2**	**2**	**3**	**2**	**2**	**3**	**3**	**2**	**3**	**2**
CO5	**3**	**3**	**3**	**3**	**2**	**3**	**3**	**3**	**3**	**3**	**2**	**3**	**2**

STRONGLY CORRELATED -3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

Sl NO	CONTENTS OF MODULE	Hrs	COs
1	**UNIT 1: PURIFICATION TECHNIQUES:** Physical properties - usefulness in analysis and methods of separation prior to analysis – Isolation techniques – extraction - crystallization, sublimation, distillation, different types of distillation techniques – steam distillation – reduced pressure distillation – fractional distillation - Analytical distillation, Thermal hazards of these techniques – chromatography – column, paper, thin layer and gas chromatography – Reaction techniques to include high dilution, vacuum line reactions, reactions aided by azeotropic distillation, recycling pyrolysis, Soxhlet extraction, continuous reactions, reactions at low temperatures, reactions in non-aqueous media and molten salts, micro quantity handling and use of glove box. Special methods in modern chemistry – methods for vacuum sublimation and quasi sublimation, technique and apparatus for reactions in inert atmosphere and under low temperature, working with compressed gases, heating under pressure, chemistry of working with hazardous materials – air/water sensitive, corrosive, toxic, explosive and radioactive materials – use of nitrogen atmosphere and its significance.	**18**	**CO1**
2	**UNIT 2: SPECTROSCOPY:** Optical spectroscopy –UV, Visible and IR spectroscopy with reference to radiation source, Optical materials, monochromators and detectors, Principles – the design of single beam and double beam spectrophotometers – Application of optical spectroscopy in qualitative and quantitative analysis 2.1 Magnetic Resonance Spectroscopy –Nuclear magnetic and electron magnetic resonance spectroscopy – Basic features of the NMR and ESR spectrometers. NMR: Chemical shift, spin-spin coupling and double resonance. NMR shift reagents – Applications of NMR spectroscopy in qualitative and quantitative analysis – wide line and FT NMR C^{13} NMR. ESR: Hyperfine splitting – g	**18**	**CO2**

	value – factors affecting the magnitude of ‘g’ value. Zero field splitting. ESR spectra of organic radicals and transition metal complexes. 2.2 Mossbauer spectroscopy–The Mossbauer effect – nuclei exhibiting Mossbauer effect – experimental techniques – isomer shift, quadrupole splitting – applications. 2.3 Photoelectron Spectroscopy –XPS and UPS- Instrumentation – radiation sources – energy analyzers and detectors – use of XPS and UPS as analytical tools **2.4** Mass spectrometry –Mass spectrometer instrumentation – the ion source, mass analysers – detectors – vacuum system – data processing – sample handling – applications of mass spectrometry in quantitative and qualitative analysis.		
3	**UNIT 3 THERMOANALYTICAL METHODS:** Thermo gravimetric analysis (TGA) Thermo balances Derivative thermo- gravimetric analysis (DTG) Differential thermal analysis (DTA) The DTA apparatus, DSC, DTA Thermometric titrations	**18**	**CO3**
4	**UNIT 4 ELECTROANALYTICAL METHODS:** a) Voltammetry: Dropping mercury electrode DME – Polarographic analysis – The shape of polarographic wave – Ilkovic equation for diffusion current – significance of half wave potentials - polarographic maxima and their eliminations – instrumentation of polarography – applications in quantitative and qualitative analysis b) Coulometry: Types of coulometric methods - coulometric analysis at constant electrode potentials – titrations involving neutralization, precipitation and complex forming reactions.	**18**	**CO4**
5	**UNIT 5 MAGNETIC PROPERTIES:**	**18**	**CO5**

	Measurements – different methods – comparison and use in structural elucidation. Magnetic susceptibility-measurement, types, applications. Temperature dependence and independence paramagnetism- Curie's law, Weiss law-ferromagnetism, ferrimagnetism, antiferromagnetism.		

References:

1. Instrumental methods of analysis, H.H.Willard, L.I. Merrit Jr and J.A.Dean. Affiliated East West Press 1974.
2. Principles of Instrumental Analysis (second edition), D.M.Scoog and D.M.West Holt-Saunders, Japan 1980.
3. Analytical Chemistry R.Gopalan, S.Chand &Co.
4. R.S.Drago, Physical methods in Inorganic Chemistry, Reinhold Ny.1968.
5. E.A.V Ebsworth, D.W.H.Rankin and S.Cradock, Structural methods in Inorganic Chemistry, Blackwell Scientific Publ., 1976.

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**CIA I**	**CIA II**	**CIA III**	**ESE**
Marks (out of 50)	**50**	**50**	**10**	**100**
Remember	20	20		40
Understand	20	20		40
Apply	10	10	5	20
Analyze			5	
Evaluate				
Create				

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	38.1
Understand	38.1
Apply	21.4
Analyse	2.4
Evaluate	
Create	

ADVANCED COURSE II
COURSE TITLE: ANALYTICAL CHEMISTRY PRACTICALS II

Course Code	**: 1923421**	**Credits**	**: 03**
L:T:P:S	**: 4:0:0:0**	**CIA Marks**	**: 40**
Exam Hours	**: 03**	**ESE Marks**	**: 60**

LEARNING OUTCOMES:

The basic understanding of various analytical techniques are being made by various analytical tools such as colorimetry, conductometry, potentiometry, UV – visible spectrophotometry, Flame photometry, cyclic voltammetry, IR and photo-catalytic reactor.

COURSE OUTCOMES: At the end of the Course, the Student will be able to

CO1	Students will use the Beer-Lambert's law and able to determine the amount of protein, Nickel and manganese by colorimetry.
CO2	Students will estimate the percentage of Sodium and Potassium in a commercial electoral sample and Sodium and Calcium in a mixture using flame photometry.
CO3	Students will use the pH meter for the determination of dissociation constant of weak acid.
CO4	Students will explain the determination of the basicity and dissociation constant of oxalic acid, phosphoric acid and acetic acid and determine the iso electric point of an amino acid by potentiometric titrations.
CO5	Students will determine the stability constant of the complex formed between potassium oxalate and lead nitrate, estimate the amount of Ascorbic acid using and verify the Randel's Sevick equation, using cyclic voltammetry.
CO6	Students will estimate the amount of Zinc by complex formation with EDTA by conductometry.
CO7	Students will verify the Beer's-Lambert's Law and calculation of Molal Extinction Coefficient at different wavelength for $KMnO_4$ and $K_2Cr_2O_7$ using UV-Visible Single beam spectrophotometer.
CO8	Students will identify functional groups in Ethyl alcohol, Acetone, Aniline, Aldehyde and Acetic acid, using Infrared Spectroscopy.

CO9	Students will determine the kinetic parameters for degradation of dye using Photo Catalytic Reactor.

MAPPING OF COURSE OUTCOMES TO PROGRAM OUTCOMES:

CO/PO/PSO	**PO**										**PSO**				
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**1**	**2**	**3**	**4**	**5**
CO1	3	3	3	3	2	2	1	3	3	3	3	2	3	2	3
CO2	3	3	3	2	3	2	1	2	2	2	3	3	2	3	3
CO3	3	3	3	3	2	2	2	2	2	3	3	2	3	3	3
CO4	3	3	3	2	3	2	2	2	2	3	3	2	3	2	3
CO5	3	3	3	3	2	3	2	2	3	3	3	3	2	3	3
CO6	3	3	3	3	3	2	3	3	2	3	3	2	3	2	3
CO7	3	3	3	3	2	3	2	3	3	2	3	2	2	3	3
CO8	3	3	3	3	2	2	2	2	2	3	3	2	3	3	3
CO9	3	3	3	3	2	3	2	2	3	3	3	3	2	3	3

STRONGLY CORRELATED - 3, MODERATELY CORRELATED – 2, WEAKLY CORRELATED -1

S.No.	CONTENTS OF MODULE	COs
  1 **2** **3**	**LIST OF EXPERIMENTS** **COLORIMETRY** Colorimetric estimation of Nickel. Colorimetric estimation of Manganese. Colorimetric estimation of protein by biuret.	**CO1**
 4 **5**	**FLAME PHOTOMETERY** Estimation of Sodium and Potassium in commercial electral samples using flame photometry. Estimation of Sodium and Calcium in a mixture using flame photometry.	**CO2**
 6	**pH METRY** Determination of dissociation constant of weak acid using pH meter.	**CO3**
 7 **8**	**POTENTIOMETRY** Determination of the basicity and dissociation constant of oxalic acid, phosphoric acid and acetic acid by potentiometry. Determination of isoelectric point of an amino acid by potentiometric titration.	**CO4**
 9 **10**	**CYCLIC VOLTAMMETRY** Determination of stability constant of the complex formed between potassium oxalate and lead nitrate using cyclic voltammetry. Estimation of Ascorbic acid using Cyclic Voltammetry. Verification of Randel's Sevick equation in Cyclic Voltammetry.	**(CO5)**
 11	**CONDUCTOMETRY** Estimation of Zinc vs EDTA by conductometry.	**CO6**
 12	**SPECTROPHOTOMETRY** Verification of Beer's-Lambert's Law and calculation of Molal Extinction Coefficient at different wavelength for $KMnO_4$ and $K_2Cr_2O_7$ using UV-Visible Single beam spectrophotometer.	**CO7**
 13	**IR-SPECTROMETER** Identification of functional groups of Ethyl alcohol, Acetone, Aniline, Aldehyde and Acetic acid, using Infrared Spectroscopy.	**CO8**
 14	**PHOTOCATALYTIC REACTOR** Determination of kinetic parameters for degradation of dye using Photo Catalytic Reactor.	**CO9**

REFERENCE BOOKS:

1. D. A. Skoog, 1985, Principles of Instrumental Methods of Analysis, III Ed.Saunders College Pubs.
2. Willard Merrit, Dean and Settle. 1986 Instrumental Methods of Analysis, VI Ed. CBS Pubs.
3. A. I. Vogel, 1976. Text Book of Qualitative Inorganic Analysis III Ed. ELBS.
4. D. A. Skoog and D. M. West, 1982 Fundamental of Analytical Chemistry, IV Ed. Old Reinhord& Winston Pubs.

ASSESSMENT PATTERN

CIE- Continuous Internal Evaluation (40 Marks)

Bloom's Category	**MODEL**	**ESE**
Marks (out of 50)	**60**	**60**
Remember		
Understand		
Apply	30	30
Analyze	30	30
Evaluate		
Create		

ESE- Semester End Examination (100 Marks; weightage 60%)

Bloom's Category	**Weightage %**
Remember	
Understand	
Apply	50
Analyse	50
Evaluate	
Create	