M.Sc. Chemistry

SYLLABUS
(Under Choice Based Credit System-CBCS)

For the Students Admitted in the Academic Year 2019-20

PG & RESEARCH DEPARTMENT OF CHEMISTRY
(DST-FIST Sponsored & DBT-STAR Scheme)
BISHOP HEBER COLLEGE (Autonomous)
(Reaccredited with ‘A’ Grade (CGPA – 3.58/4.0) by the
NAACRecognized by UGC as “College of Excellence”
TIRUCHIRAPPALLI – 620 017

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PG & Research Department of Chemistry

Bishop Heber College (Autonomous), Trichy -17

Vision:

The PG & Research Department of Chemistry envisions…

To transform students into globally-competent graduates by providing a vibrant, Innovative and all-inclusive learning environment that fosters Values, Professional ethics and Social Consciousness.

Mission:

To reach its vision the Department would

- offer a Quality and Comprehensive Curriculum
- facilitate a Competent Learning Environment
- create an Integrated Research Culture
- foster Industry – Academia Network for education
- inspire to Innovate

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Program Outcomes – M.Sc. Chemistry

On successful completion of the M.Sc. Chemistry program, the post graduand will be able toexhibit the following abilities in the respective domains.

KNOWLEDGE

PO1: Exhibit substantial and advanced knowledge in Organic, Inorganic, Physical and related fields of Chemistry.

PO2: Apply concepts and theories of chemistry to solve qualitative and quantitative problems

PO3: Disseminate scientific and technical information to both Professional and broader audience effectively.

SKILLS

PO4: Analyze complex problems through appropriate techniques, experiments, computational tools, spectral and instrumental methods to provide solutions.

PO5: Assess experimental and research problems critically and independently to arrive at objective conclusions.

PO6: Exhibit digital proficiency in data analysis, library search, basic chemistry software and related computational tools.

ATTITUDES

PO7: Contribute to diverse teams through leadership and collaborative skills and hence adaptable to Jobs in Chemical industries, Academic institutions, Research organizations, corporate and public sectors.

ETHICAL & SOCIAL VALUES

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PO8: Practice professional and ethical values with a consciousness to legal, environmental and social responsibilities in all walks of life.

PO9: Observe IPR guidelines while designing, documenting and publishing a possible project.

Program Specific Outcomes - M. Sc. Chemistry

On Successful Completion of M.Sc. Chemistry program, graduand would have acquired thefollowing competencies:

Knowledge & Skills Domain

PSO1 : Relate the properties, reactions and applications of various chemical entities using theories and principles.

PSO2: Evaluate the various reaction mechanisms to plan synthetic routes and choose the right modus operandi for reactions and processes in laboratory with safety and environmental security.

PSO3: Comprehend the mathematical and physical basis of the behaviour of chemical speciesand processes.

PSO4: Develop analytical skills and problem solving skills in addition to project based

PROGRAM ARTICULATION MATRIX - M.Sc. CHEMISTRY

S. No	Name of the Course	Course Code	CORRELATION WITH PROGRAM OUTCOMES AND PROGRAM SPECIFIC OUTCOMES												
			PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PSO1	PSO2	PSO3	PSO4
1	Bonding & Structure of Inorganic Compounds	P19CH101	M	M	M	M	L	-	M	-	M	H	H	L	H
2	Concepts in Organic Chemistry	P19CH102	H	H	M	M	M	-	L	L	L	H	M	L	M
3	Chemical Kinetics & Quantum Mechanics	P19CH103	H	M	M	H	H	-	M	M	-	H	M	H	M
4	Inorganic Quantitative Estimations & Complex Preparation	P19CH1P1	M	H	M	H	H	M	H	M	L	H	M	M	H
5	Organic Synthesis & Separation Techniques	P19CH1P2	H	H	H	H	H	L	H	M	L	H	M	M	H
6	Coordination & Organometallic Chemistry	P19CH204	M	M	L	L	L	M	L	M	-	M	M	L	-
7	Reactions & Mechanisms In Organic Chemistry	P19CH205	H	H	H	M	H	L	M	-	M	H	H	M	M
8	Inorganic Semimicro Analysis & Colorimetric Estimations	P19CH2P3	M	H	M	M	M	L	M	M	L	H	H	M	H
9	Quantitative Analysis of Organic Compounds	P19CH2P4	H	H	H	H	H	-	H	M	H	H	H	M	H
10	Data Analysis & Selected Analytical	P19CH2:1	H	H	M	H	M	M	L	M	H	M	L	H	H

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	Techniques														
11	RI / MI	P17VL2:1/ P17VL2:2													
12	Organic Spectroscopy	P19CH306	H	H	M	H	M	-	M	M	M	H	H	H	H
13	Thermodynamics & Electrochemistry	P19CH307	M	M	L	L	L	-	-	-	-	M	-	M	L
14	Physical Chemistry Practical (Non Electrical)	P19CH3P5	H	H	M	M	H	-	M	H	-	H	H	H	M
15	Physical Chemistry Practical (Electrical)	P19CH3P6	H	H	M	H	H	L	L	L	L	H	M	M	H
16	Bio-Inorganic Chemistry	P19CH3:2	M	M	M	M	M	-	-	M	-	M	M	M	L
17	Project	P19CH4PJ													
18	Inorganic Spectroscopy	P19CH408	H	M	L	M	M	L	M	L	L	H	M	M	M
19	Group Theory & Spectroscopy	P19CH409	L	M	M	M	M	M	L	L	L	M	M	M	M
20	Applications of Drug Design & Discovery	P19CH4:3	M	M	M	H	M	M	L	L	L	H	M	L	L
21	Selected Topics in Chemistry	P19CH4:4	M	M	M	M	L	L	H	L	L	M	M	M	M
22	Computer Aided Molecular Calculations	P19CH4:P	M	M	L	M	M	H	-	-	-	L	-	L	M
23	Project	P19CH4PJ	H	M	H	M	H	H	M	M	M	H	H	L	M

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PG& RESEARCH DEPARTMENT OF CHEMISTRY

Structure of the Curriculum-M.Sc. Chemistry

Semester - I			Semester - II		
	Hours	**Credits**		**Hours**	**Credits**
Core Theory - 1	6	6	Core Theory - 4	6	6
Core Theory - 2	6	6	Core Theory - 5	6	6
Core Theory - 3	6	6	Core Practical - 3 (Lab. Cum Theory)	5	3
Core Practical - 1 (Lab. Cum Theory)	6	3	Core Practical - 4 (Lab. Cum Theory)	6	3
Core Practical - 2 (Lab. Cum Theory)	6	3	Elective - 1	5	4
			VLO - 1	2	2
Total	**30**	**24**	**Total**	**30**	**24**
Semester - III			**Semester - IV**		
	Hours	**Credits**		**Hours**	**Credits**
Core Theory - 6	6	5	Core Theory - 8	6	5
Core Theory - 7	6	5	Core Theory - 9	6	5
Core Project Preparatory Course	1	-	Core Project	5	4
Core Practical - 5	6	3	Elective - 3	5	4
Core Practical - 6 (Lab. Cum Theory)	6	3	Elective - 4	5	2
Elective - 2	5	4	Elective - 5 : Practical	3	2
Total	**30**	**20**	**Total**	**30**	**22**

Total	**120 Hours**	**90 Credits**

PARTS OF THE CURRICULUM	NO. OF COURSES	CREDITS
Core Course (Theory)	9	50
Core Course (Practical)	6	18
Elective	5	16
Project	1	4
VLO	1	2
TOTAL	22	90

**** INTERNSHIP**

- **2 Extra credits** can be earned by attending Summer/ Winter Internship on submission of attendance certificate for a period of 8 weeks with a Project Report.
- **Industrial Visit** to Chemical Industries, Pharmaceutical Industries, CSIR-Centres, Sophisticated Instrumentation Centres etc., within India and submission of Mini Report is also entertained .

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Structure of the Curriculum (PG Chemistry)

Sem	Course	Course Code	Course Title	Hrs/ Week	Credits	MARKS		
						CIA	ESA	TOTAL
I	Core I	P19CH101	Bonding & Structure of Inorganic Compounds	6	6	25	75	100
	Core II	P19CH102	Concepts in Organic Chemistry	6	6	25	75	100
	Core III	P19CH103	Chemical Kinetics & Quantum Mechanics	6	6	25	75	100
	Core Practical I	P19CH1P1	Inorganic Quantitative Estimations & Complex Preparation	6	3	40	60	100
	Core Practical II	P19CH1P2	Organic Synthesis & Separation Techniques	6	3	40	60	100
II	Core IV	P19CH204	Coordination & Organometallic Chemistry	6	6	25	75	100
	Core V	P19CH205	Reactions & Mechanisms In Organic Chemistry	6	6	25	75	100
	Core Practical III	P19CH2P3	Inorganic Semimicro Analysis & Colorimetric Estimations	5	3	40	60	100
	Core Practical IV.	P19CH2P4	Quantitative Analysis of Organic Compounds	6	3	40	60	100
	Elective-I	P19CH2:1	Data Analysis & Selected Analytical Techniques	5	4	25	75	100
	VLO	P17VL2:1/ P17VL2:2	RI / MI	2	2	25	75	100
III	Core VI	P19CH306	Organic Spectroscopy	6	5	25	75	100
	Core VII	P19CH307	Thermodynamics & Electrochemistry	6	5	25	75	100
	Core Practical V	P19CH3P5	Physical Chemistry Practical (Non Electrical)	6	3	40	60	100
	Core Practical VI	P19CH3P6	Physical Chemistry Practical (Electrical)	6	3	40	60	100
	Elective -II	P19CH3:2	Bio-Inorganic Chemistry	5	4	25	75	100
	Core Project	P19CH4PJ	Project	1	-			
IV	Core VIII	P19CH408	Inorganic Spectroscopy	6	5	25	75	100
	Core IX	P19CH409	Group Theory & Spectroscopy	6	5	25	75	100
	Elective III	P19CH4:3	Applications of Drug Design & Discovery	5	4	25	75	100
	Elective IV	P19CH4:4	Selected Topics in Chemistry	5	2	25	75	100
	Elective V-Practical	P19CH4:P	Computer Aided Molecular Calculations	3	2	40	60	100
	Core Project	P19CH4PJ	Project	5	4	--	--	100
Total				**120**	**90**			**2200**

Elective Optional Papers

1. Green Chemistry
2. Radiation Chemistry
3. Chemistry of Polymers
4. Analytical Techniques in Chemistry
5. Natural Products Chemistry

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Course - I: **BONDING AND STRUCTURE OF INORGANIC COMPOUNDS**

Semester : 1 **Course Code : P19CH101**
Credits : 6 **Total Hrs : 90**
Hours /Week:6

1. Course Outcomes:

At the end of this course, the students will be able to

S.No.	Course Outcomes	Level	Unit
1	Predict the reactivity of chemical compounds based on acid-base concepts and HSAB principle	K5	I
2	Assess the role of non-aqueous solvents in chemical reactions	K5	I
3	Distinguish different types of crystal structures and crystal defects	K5	II
4	Explain the nuclear properties, stability and applications of radioactive nuclei	K4	III
5	Predict the structure, geometry, optical and electronic properties of inorganic Compounds using VB, VSEPR, MO and Band theories	K5	IV
6	Classify electron deficient, electron precise and electron rich inorganic compounds based on their structure and bonding	K4	V

2A. Syllabus

UNIT-I SOLVENTS 18 HOURS

1 .1 Acids and Bases

Differentiating and levelling solvents – Usanovich and Lux Flood concepts – Solvent ion theory of acids and bases –Hard and Soft Acids and Bases (HSAB)– Classification, acid-base strength and hardness and softness – Symbiosis – Theories of hardness and softness – Electronegativity and hardness and softness – Applications of HSAB, Proton sponges.

1.2 Non-aqueous solvents: Classification- protic and aprotic solvents, – Liquid NH_3, BrF_3, CH_3COOH, liquid SO_2, liquid HF. Proton sponges- molten salts as solvents and ionic liquids.

UNIT–II IONIC BONDING AND CRYSTAL STRUCTURE 18 HOURS

2.1 Packing of ions in crystals & crystal structure – ccp, hcp, bcc, fcc

2.2 Radius ratio and structure of ionic lattices, Calculation of radius ratio and Coordination No, stoichiometry and crystal structures of NaCl, CsCl, Zincblende, wurtzite, Rutile, Flourite, antifluorite, perovskite, CdI_2, β- cristobalite & ReO_3 structure, Spinels Inverse Spinels.

2.3 Lattice energy- Slater’s rule, Born-Haber cycle- Born-Lande equation, Factors affecting Lattice Energy

2.4 Crystal defects: Stoichiometric and non- stoichiometric defects. Metal excess defects – Metal deficiency defects - calculation of number of defects.

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UNIT-III NUCLEAR CHEMISTRY 18 HOURS

3.1 Nuclear Chemistry

The Structure of the nucleus, Radioactive equilibrium, Orbital electron capture, Nuclear isomerism, Internal conversion, Nuclear cross section.

Nuclear stability- Binding energy, shell model, magic numbers, Harkin's rule, Theories of decay processes-Geiger-Nuttal rule, Group displacement laws and units of radioactivity

3.2 Radioactivity

Nuclear reactions: Q- value of nuclear reactions, transmutation, stripping and pickup, fission, fusion, spallation, projectile capture and particle emission reaction, fragmentation and scattering.

Particle accelerators: Cyclotron, linear accelerator and synchrotron

Nuclear reactors: Power reactor, breeder and Fast breeder reactors

Radioactive techniques:Tracer technique, Neutron activation and Isotopic dilution analysis.

Counting techniques: Geiger-.Muller, scintillation and proportional counters.

Applications: carbon dating, agriculture, medicine and industry.

UNIT-IV COVALENT BONDING 18 HOURS

4.1 VBT: Resonance, conditions for resonance, formal charges, hybridization and geometry, VSEPR model- CH_4, NH_3, H_2O, PCl_3F_2 - Bents' rule and Walsh diagram- SF_4, BrF_3, ICl_2^-, ICl_4^-, XeF_4, $XeOF_4$, XeO_4, XeO_3, XeF_6, XeF_2

4.2 MOT: LCAO method- MO level energy level diagram of hetero diatomic molecule HCl) and polyatomic molecule NH_3 and SF_6–LUMO and HOMO concepts in bonding.

4.3 Bonding in metals: Band theory of solids, Insulators, Semiconductors- n and p type, Super conductors and its applications.

UNIT-V INORGANIC CHAINS, RINGS & CAGES COMPOUNDS 18 HOURS

5.1 Electron deficient , electron precise and electron rich compounds: **Boranes and carboranes**: Structure of B_2H_6 , B_4H_{10}, $B_{12}H_{12}^{2-}$,B_6H_{10}, B_8H_{12}, $B_{10}H_{14}$. Synthesis of neutral boron hydrides, polyhedral boron anions and dianions, structure of polyhedral boranes-nido – arachno- and closo – frameworks, PSEPT (Wade's rule and Styx code). Carboranes- synthesis, polyhedral geometries of metalloboranes and metallocarboranes.

5.2 Boron –Nitrogen compounds:

Structure and bonding of $B_3N_3H_6$, Borazines, B-N clusters and azaboranes.

5.3 Metal clusters: Structure and bonding of dinuclear cluster $Re_2Cl_8^{2-}$

5.4 Poly acids: Structure of isopoly and heteropoly anions and polycations of W and Mo.

5.5 P-N and P-S compounds: Polyphosphazene, cyclophosphazene, P-S cages.

5.6 Cyclic S-N compounds: Tetra sulphur –tetranitride (S_4N_4) and Polythiazyl.

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2B.Topics for Self-Study:

S.No.	Topics	Web Links
1	Acid base Equilibrium	https://www.youtube.com/watch?v=jdmHjFp_35I
2	Crystal structure Review	https://www.youtube.com/watch?v=iPb8vRtroLU
3	Nuclear Radiation	https://www.youtube.com/watch?v=iTb_KRG6Lxo
4	Bonding in metal carbonyls	https://www.youtube.com/watch?v=ZkSuggOV9dA
5	cluster of compounds	https://www.youtube.com/watch?v=LHevfXFKl_E

2C.Text Books

1. James E. Huheey, Ellen A Keiter and Richard L. Keiter, “Inorganic Chemistry: Principles of Structure and Reactivity”, Pearson Education, India, 2014. **(Unit- I, II, IV, V)**

2. H.J. Arnikar, “Essentials of Nuclear Chemistry”, New Age International, 2011. **(Unit- III)**

2D.Reference Books

1. Bodie E. Douglas and Darl H. Mc Daniel, John J. Alexander, “Concepts and Models in Inorganic Chemistry”, Wiley Eastern, New Delhi, 2006.
2. J.D. Lee, “Concise Inorganic Chemistry”, Oxford University Press, New Delhi, 2008.
3. Keith F. Purcell and John C. Kotz, Inorganic Chemistry, Saunders Golden Sunburst Series, E.B. Saunders Company, Philadelphia, 2010.
4. F.Albert Cotton, Geoffrey Wilkinson and Carlos A. Murillo, “Advanced Inorganic Chemistry”, John Wiley and Sons, Singapore, 2007.
5. B.R. Puri, L.R. Sharma and K.C. Kalia “Principles of Inorganic Chemistry” – Vishal Publishing Co., Jalandhar, 2017.
6. S. Glasstone, “Source Book on Atomic Energy” – 3rd Edition, Affiliated East-West Press Pvt. Ltd., New Delhi, 2014.
7. Gary L. Miessler, Donald A. Tarr, “Inorganic Chemistry”, Pearson Education, New Delhi, 2008.

3.Specific Learning Outcomes (SLO)

Unit	Course Content	Learning Outcomes	Blooms Taxonomic levels of Transaction
	Unit – 1:		
1.1	Differentiating and leveling solvents.	Distinguish the differentiating and leveling solvents.	K2
	Usanovich, Solvent ion theory of acids and bases and Lux-Flood concepts.	Apply the concepts of acid and bases and identify inorganic species as acids or bases.	K3
	Hard and Soft Acids and Bases (HSAB)– Classification, electronegativity, acid-base strength and hardness and softness.	classify inorganic compounds as hard and soft using the principle of HSAB and to correlate electronegativity, acid-base strength and hardness and softness.	K4
	Applications of HSAB concept.	Interpret the various applications of hardness and softness.	K5
1.2	**Non aqueous solvents:** Classification - protic and aprotic solvents.	Classify various solvents.	K4
	Liquid NH_3, BrF_3, CH_3COOH, liquid SO_2, liquid HF.	Explain the chemistry of different non-aqueous solvents.	K5
	Proton sponges - molten salts as solvents and ionic liquids.	Examine the characteristics of ionic liquids and proton sponges.	K4
	Unit – 2:		
2.1	Packing of ions in crystals Crystal structure – ccp, hcp, bcc, fcc.	Classify the different types of packing and crystal structure.	K4

2.2	Radius ratio and structure of ionic lattices, Calculation of radius ratio and Coordination No.	Calculate radius ratio, structure of ionic lattices and coordination number by applying the radius ratio rule.	K4
	Stoichiometry and crystal structures of NaCl, CsCl, Zinc blende Wurtzite, Rutile, Flourite, Antifluorite, Perovskite, CdI_2, β-cristobalite & ReO_3 structure.	Justify the stoichiometry in different types of crystal structures	K5
	Spinels and Inverse Spinels.	Contrast the structure and stochiometry of Spinels and Inverse Spinels.	K4
2.3	Lattice energy- Slater's rule Born-Haber cycle - Born-Lande equation, Factors affecting Lattice Energy.	Calculate lattice energy using Slater's rule and Born-Haber cycle and illustrate the factors affecting Lattice Energy.	K4
2.4	Crystal defects: Stoichiometric and non stoichiometric defects. Metal excess defects – Metal deficiency defects, Calculation of number of defects.	Distinguish the different types of crystal defects.	K4
		Estimate the defects in the stoichiometric and non-stoichiometric crystals.	K5
	Unit – 3:		
3.1	**Nucleus**- Structure of the nucleus.	Analyze the structural components of an atomic nucleus.	K4
	Radioactive equilibrium, Orbital electron capture, Nuclear isomerism, Internal conversion, Nuclear cross section.	Compare the different types of nuclear reactions.	K4
	Nuclear stability- Binding energy, shell model, magic numbers, Harkin's rule.	Deduce the stability of nucleus based on binding energy, n/p ratio.	K5
	Theories of decay processes - Geiger-Nuttal rule, Group displacement laws and units of radioactivity.	Examine the theories of decay processes.	K4
3.2	**Nuclear reactions**: Q- value of nuclear reactions, transmutation, stripping and pickup, fission, fusion, spallation, projectile capture and particle emission reaction, fragmentation and scattering.	Calculate the Q- value of nuclear reactions and to differentiate the nuclear transmutation reactions.	K4

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	Particle accelerators: Cyclotron, linear accelerator and synchrotron **Nuclear reactors**: Power reactor, breeder and Fast breeder reactors.	Compare and contrast the working and applications of different types of particle accelerators.	K4
	Radioactive techniques: Tracer technique, Neutron activation and Isotopic dilution analysis.	Explain the importance, working and applications of radioactive techniques.	K4
	Counting techniques: Geiger-.Muller, scintillation and proportional counters.	Illustrate the different techniques used to quantify ionising radiations.	K4
	Applications: Carbon dating, agriculture, medicine and industry.	Calculate the age of antique material by carbon dating and explain the role of radioactive materials in agriculture, biology, industry and pharmaceuticals.	K4
	Unit - 4:		
4.1	**VBT**: Resonance, conditions for resonance, formal charges Hybridization and geometry: VSEPR model - CH_4, NH_3, CH_3^+, NH_4^+, SO_4^{2-}, CO_3^{2-}, H_2O, PCl_3F_2 . Bents' rule- SF_4, BrF_3, ICl_2^-, ICl_4^-, XeF_4, $XeOF_4$, XeO_4, XeO_3, XeF_6, XeF_2.	Predict the structure, hybridization and geometry of inorganic molecules using VSEPR and VB theories.	K5
4.2	**MOT:** LCAO method MO level energy level diagram of hetero diatomic molecule (HCl) and polyatomic molecule NH_3 and SF_6 – LUMO and HOMO concepts in bonding.	Explain the type of bonding in poly atomic molecules using HOMO and LUMO concepts of MOT.	K4
4.3	**Bonding in metals:** Band theory of solids.	Analyze the optical and electronic properties of semiconductors using Band theory of solids.	K4
	Insulators, Semiconductors n and p type, Super conductors and its applications.	Compare the different types of semiconductors and list their applications.	K4
	Unit – 5:		
5.1	**Electron deficient , electron precise and electron rich compounds**:		

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	Boranes and Carboranes: Structure of B_2H_6 ,B_4H_{10}, $B_{12}H_{12}^{2}$, B_6H_{10}, B_8H_{12}, $B_{10}H_{14}$. Synthesis of neutral boron hydrides, polyhedral boron anions and dianions. PSEPT (Wade's rule and Styx code).	Predict the type of boranes and carboranes based on Wade's rule and Styx code.	K5
	Structure of polyhedral boranes - nido–arachno and closo–frameworks.	Explain the classification and structure of polyhedral boranes.	K4
	Carboranes - synthesis, polyhedral geometries of metalloboranes and metallocarboranes.	Explain the synthesis and structure and bonding in Carboranes.	K4
5.2	**Boron –Nitrogen compounds**: Structure and bonding of B3N3H6, Borazines, B-N clusters and azaboranes.	Examine the structure and bonding of Boron –Nitrogen compounds.	K4
	Metal clusters: Structure and bonding of dinuclear cluster Re $_{2}Cl_{82}$.	Analyze the structure and bonding of Metal clusters.	K4
	Poly acids: Structure of isopoly and heteropoly anions and polycations of W and Mo.	Inspect the structure and bonding of Structure of isopoly and heteropoly anions.	K4
	P-N and P-S compounds: Polyphosphazene, cyclophosphazene, P-S cages.	Correlate the structure and bonding of the P-N and P-S compounds.	K4
	S-N compounds: Tetra sulphur – tetranitride (S_4N_4) and Polythiazyl.	Illustrate the different types of S-N compounds.	K4

4. Mapping Scheme for the PO, PSOs and Cos

L-Low M-Moderate H- High

Course Title: BONDING AND STRUCTURE OF INORGANIC COMPOUNDS **Course Code : P19CH101**													
Mapping	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PSO1**	**PSO2**	**PSO3**	**PSO4**
CO1	M	H	M	M	H	-	-	-	-	H	H	-	H
CO2	L	M	M	M	M	-	M	-	M	H	M	-	M
CO3	M	-	M	M	L	-	-	-	M	M	L	-	H
CO4	M	M	M	M	L	-	-	-	-	-	L	-	H
CO5	M	H	M	M	L	-	M	-	-	M	H	-	H
CO6	H	M	-	M	M	-	M	-	-	H	M	L	H

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5.Course Assessment Methods

Direct

1. Continuous Assessment Test (Model Exams) I,II
2. Open book test; Cooperative learning report, Assignment; Journal paper review, Group Presentation, Project report, Poster preparation, Proto-type or Product Demonstration etc. (as applicable)
3. End Semester Practical Examination

Indirect

1. Course-end survey

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Core Course: II **CONCEPTS IN ORGANIC CHEMISTRY**

Semester : 1 **Code : P19CH102**
Credits : 6 **Total Hrs :90**
Hours /Week:6

1.Course Outcomes:

After the successful completion of this course the students will be able to

S.No.	Course Outcomes	Level	Unit
1	Apply the rules of nomenclature to name organic compounds	K3	I
2	Distinguish the reactive intermediates and factors affecting their stability	K5	II
3	Examine the evidences for the kinetics and thermodynamic aspects of reactions	K4	II
4	Apply Huckle's and Craig's rules of aromaticity to benzenoid and non-benzenoid compounds	K3	III
5	Categorize the organic compounds based on stereochemistry	K4	IV
6	Evaluate different methods of reaction mechanism related to molecular rearrangements	K5	V

2A. Syllabus

UNIT– I NOMENCLATURE OF ORGANIC COMPOUNDS 18 Hours

1.1 Nomenclature :– General rules-Naming of linear and branched alkanes, alkenes, polyenes and alkynes with two or three functional groups by IUPAC nomenclature. Aromatic and heteroaromatic systems- nomenclature of heterocycles having not more than two hetero atoms such as oxygen, nitrogen and sulphur. Fused heterocycles and fused aromatic systems.

1.2 Nomenclature of alicyclic, bicyclic and tricyclic compounds- organic molecules including regio and stereoisomers.

UNIT–II REACTION MECHANISMS AND INTERMEDIATES 18 Hours

2.1 Reaction Mechanism: Structure and Reactivity:-Types of reactions, Types of mechanisms, Rate constants – determination and life times of reactive energy states -. Potential energy diagrams, transition states and intermediates, methodsof determining mechanisms, isotope effects. Thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

2.2 Reactive Intermediates:-Free radicals, carbenes, nitrenes, carbanions, classical and non-classical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations.

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UNIT–III AROMATICITY OF ORGANIC COMPOUNDS 18 Hours

3.1 Aromaticity-: Electron delocalization and resonance -Huckel's rule-Aromaticity in benzenoid and non- benzeneoid compounds, alternant and non-alternant hydrocarbons- Craigs rule (fused ring system)- Aromaticity on larger annulenes- antiaromatic - homoaromatic and non-aromatic compounds -Molecular orbital description of aromaticity and anti aromaticity.

3.2 Some Selected reactions of aromatic system :-Electrophilic aromatic substitution***:*** Gattermann reaction - Gattermann- Kosch formylation reaction- Hoeben- Hoesch reaction- Vilsmeyer formylation. *Nucleophilic aromatic substitution:* Chichibabin amination - Bucherer reaction. *Transition metal chemistry:* Pauson-Khand reaction- Heck reaction-Suzuki Coupling -Stille Coupling - Sonogashira Coupling- Negishi cross coupling.

UNIT –IV ORGANIC STEREO CHEMISTRY 18 Hours

4.1 Optical Isomerism - ***Brief introduction to Chirality:*** Asymmetry- dissymmetry -chiral axis and chiral planes- examples (Biphenyls, Allenes, spiranes and ansa compound, cyclophanes respectively). ***Prochirality:*** Principles of Stereogenecity, stereoselectivity, enantioselectivity, diastereoselectivity. Enantiotopic and Diasterotopic. ***Asymmetric synthesis***: Stereoselective and stereospecific synthesis - stereochemical aspects through various models (Cram / Cram chelation / Felkin-Anh models); Cram's rule. ***Methods of resolution:*** crystal growth-enantiomeric excess.

4.2 Dynamic stereochemistry -Conformational analysis -Introduction to terms - conformers, configuration, dihedral angle, torsional strain, conformations. Conformational analysis of cycloalkanes (3,4,5 and 6 membered ring with two substituents). Winstein Eliel equation- Curtin-Hammet principle.

UNIT-V MOLECULAR REARRANGEMENT 18 Hours

5.1 ***Migration of Carbon:*** Wagner-Meerwein rearrangement-Wolf rearrangement-Benzil benzilic acid rearrangement, ***Migration to electron deficient nitrogen:*** Hofmann rearrangement – Beckmann rearrangement- Schimdt rearrangement. ***Migration to electron deficient oxygen:*** Bayer Villager oxidation- Dakin reaction.

5.2 ***Migration to electron rich carbon :*** Favorskii rearrangement – Stevens rearrangement- Wittig rearrangement. Neber rearrangement. ***Other rearrangements:*** Dienone-phenol rearrangement - Benzidine rearrangement – Gruvenstein and Zimmermann rearrangements.

2B.Topics for Self Study

S. No	Topics	Web links
1	Nomenclature of polycyclic systems	https://www.acdlabs.com/iupac/nomenclature/79/r79_164.htm https://www.acdlabs.com/iupac/nomenclature/79/r79_166.htm http://publications.iupac.org/pac/1999/pdf/7103x0513.pdf https://doi.org/10.1007/978-3-662-01665-7_1
2	Reaction mechanism and intermediates	https://en.wikipedia.org/wiki/ANRORC_mechanism https://synarchive.com/named-reactions/zincke-reaction

		https://www.organic-chemistry.org/namedreactions/fukuyama-coupling.shtm
3	Aromaticity and related reactions	https://chemistry.illinois.edu/system/files/inline-files/02JanowiczFINALAbstract.pdf http://www.f.u-tokyo.ac.jp/~kanai/seminar/pdf/Lit_K_Yamamoto_M1.pdf https://www.organic-chemistry.org/namedreactions/chan-lam-coupling.shtm
4	Optical Isomerism	https://www.sparknotes.com/chemistry/organic2/carbocycles/section3/ https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Book%3A_Basic_Principles_of_Organic_Chemistry_(Roberts_and_Caserio)/12%3A_Cycloalkanes_Cycloalkenes_and_Cycloalkynes/12.09%3A_Conformations_of_Decalin https://www.chemtube3d.com/stdecalins/ http://www.mpgpgcollegehardoi.in/Decalins.pdf https://www.chemistry.mcmaster.ca/silicone/SharplessEdited.pdf
5	Molecular Rearrangements	https://www2.chemistry.msu.edu/faculty/reusch/virttxtjml/rearang2.htm#top1 http://burton.chem.ox.ac.uk/handout-2-2018.pdf https://pubs.acs.org/doi/10.1021/ar700198z

2C.Text Books

1. R. Panico, W.H. Powell, L. Jean,C. Richer, “A Guide of IUPAC Nomenclature of Organic compounds” , Wiley-Blackwell, 1993. **(Unit-I)**
2. Jerry March, “Advanced Organic Chemistry – Reaction Mechanisms and Structure”, Wiley India, 2006. **(Unit-II, III)**
3. D. Nasipuri “Stereochemistry of Organic Compounds”, New Age International, New Delhi, 2018. **(Unit-IV)**
4. P.S. Kalsi, “Stereochemistry, Conformations and Mechanism”, New Age International Private Limited, New Delhi, 2017. **(Unit-IV)**
5. Ahluwalia V K, “Organic Reaction Mechanism” Narosa Publication, 2010. **(Unit-V)**
6. S.M. Mukherji and S.P.Singh, “Reaction Mechanism in Organic Chemistry”, Macmillan India Ltd., Patna, 1990. **(Unit-V)**

2D.Reference Books

1. R.S. Cahn and O.C. Dermer, “Introduction to Chemical Nomenclature”, Butterworths, London, 1979.
2. Peter Sykes, “A Guide Gook to Mechanism in Organic Chemistry”, Pearson Education, New Delhi, 2003.
3. E.L. Eliel, “Stereochemistry of Carbon Compounds”, McGraw Hill, New Delhi, 2003.
4. Jonathan Clayden, Nick Greeves, Stuart Warren, “Organic Chemistry”, Oxford University Press, 2014.

Xxxx- Revised content

3.Specific Learning Outcomes (SLO)

Unit	Course Contents	Learning Outcomes	Blooms Taxonomic Highest Level of Transaction
	Unit – 1 : Nomenclature of Organic Compounds		
1.1	**Nomenclature**–General rules-Naming of linear and branched alkanes,alkenes, polyenes and alkynes with two or three functional groups by IUPAC nomenclature	Apply IUPAC rules to name compounds • with two / three functional groups	K3
	Aromatic and heteroaromatic systems-nomenclature of heterocycles having not more than two hetero atoms such as oxygen, nitrogen and sulphur. Fused heterocycles and fused aromatic systems.	Apply IUPAC rules to name compounds • heterocycles having not more than two hetero • Fused heterocycles and fused aromatic systems	K3
1.2	Nomenclature of alicyclic, bicyclicand tricyclic compounds- organic molecules including region and stereoisomers.	Apply IUPAC rules to name compounds of bicyclic and tricyclic compounds- organic molecules including region and stereoisomers.	K3
	Unit- 2: Reaction Mechanisms and Intermediates		
2.1	Types of reactions, Types of mechanisms, Rate constants – determination and life times of reactive energy states -. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects.	Distinguish Intermediates and Transition state.	K4
		Illustrate methods of determining mechanism.	K4
		Evaluate different types of mechanism.	K4
	Thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Quantitative treatment. The Hammett equation and linear free energy relationship, substituent and	Illustrate how reactions proceeds, kinetics and thermodynamics of reactions mechanisms including Hammond's postulate	K4

	reaction constants. Taft equation	To apply Quantitative Measurement of Substituent Effects on Chemical Reactivity - Hammett equation and Taft equation and their significances	K3
2.2	**Reactive Intermediates** Free radicals, carbenes, nitrenes, carbanions, classical and non-classical, carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations	Compare the different reactive intermediates and various factors affecting their stability, the rearrangements associated with such intermediates	K4
		Apply of NMR spectroscopy in the detection of carbocation	K3
	Unit – 3: Aromaticity of Organic Compounds		
3.1	**Aromaticity** Electron delocalization and resonance - Huckel's rule- Aromaticity in benzenoid and non-benzenoid compounds, alternant and non- alternant hydrocarbons-	Apply Huckles rules of aromaticity and use that to identify aromaticity / anti aromatcity / non aromaticity in benzenoid and non benzenoid compounds	K3
		Compare alternante and non - alternante hydrocarbons-	K2
	Craigs rule (fused ring system)- Aromaticity on larger annulenes- antiaromatic - homoaromatic and non-aromatic compounds -	Apply Craig's rules of aromaticity to identify aromaticity in benzenoid and non benzenoid compounds	K3
	Molecular orbital description of aromaticity and anti aromaticity.	Determine aromatic compounds and anti-aromatic compound based on Molecular orbital description.	K3
3.2	**Some Selected reactions of aromatic system** ***Electrophilic aromatic substitution:*** Gattermann reaction - Gattermann-Kosch formylation reaction- Hoeben-Hoesch reaction- Vilsmeyer formylation. ***Nucleophilic aromatic substitution:*** Chichibabinamination – Bucherer reaction. ***Transition metal chemistry:*** Pauson-Khand reaction-Heck reaction-Suzuki Coupling -Stille Coupling - Sonogashira Coupling-Negishi cross coupling.	Explain the mechanism of various aromatic electrophilic/ nucleophilic substitution reaction for synthetic applications.	K3
		Predict different aromatic electrophilic substitution reaction.	K3

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	Unit- 4: Organic Stereo Chemistry		
4.1	***Brief introduction to Chirality:*** Asymmetry- dissymmetry -chiral axis and chiral planes- examples (Biphenyls, Allenes, spiranes and ansa compound, cyclophanes respectively). ***Prochirality:*** Principles of Stereogenecity, stereoselectivity, enantioselectivity, diastereoselectivity. Enantiotopic and Diasterotopic. ***Asymmetric synthesis***: Stereoselective and stereospecific synthesis - stereochemical aspects throughvarious models (Cram / Cram chelation /Felkin-Anh models); Cram's rule. ***Methods of resolution:*** crystal growth-enantiomeric excess	Examine chirality of compounds without chiral centers [Allens , Biphenyls, spiranes, ansa compounds and cyclophanes]	K4
		Deduce Asymmetric synthesis, Stereo selective and stereospecific synthesis – for synthetic applications	K4
		Apply Cram / Cram chelation /Felkin-Anh models for asymmetric synthesis	K3
		Predict various re arrangement reactions /their mechanism and their importance in synthesis	K3
		Illustrate how seeding method can be employed for the resolution of enantiomers	K3
4.2	**Dynamic stereochemistry -** Conformational analysis **-**Introduction to terms - conformers, configuration, dihedral angle, torsional strain, conformations. Conformational analysis of cycloalkanes (3,4,5 and 6 membered ring with twsubstituents). WinsteinEliel equation-Curtin-Hammet principle.	Analyze the stability cycloalkanes of 3,4,5 and 6 membered ring with two substituents using conformational analysis Using WinsteinEliel equation-Curtin-Hammet principle to arrive at the product ratio in a chemical reaction	K4
	Unit - 5 Molecular rearrangement		

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5.1	Migration of Carbon: Wagner-Meerwein rearrangement-Wolf rearrangement-Benzil benzilic acid rearrangement, Migration to electron deficient nitrogen: Hofmann rearrangement – Beckmann rearrangement- Schimdt rearrangement. Migration to electron deficient oxygen: Bayer Villager oxidation- Dakin reaction.	Predict the products of different rearrangement reactions with mechanistic details	K5
5.2	Migration to electron rich carbon : Favorskii rearrangement – Stevens rearrangement-Wittig rearrangement. Neber rearrangement. Other rearrangements: Dienone-phenol rearrangement - Benzidine rearrangement – Gruvenstein and Zimmermann rearrangements.	Analyze the role of the Migrating groups in the rearrangement reactions	K4
		Explain based on evidences, the plausible mechanisms of rearrangements	K4

4.Mapping Scheme for the PO, PSOs and Cos

L-Low M-Moderate H- High

Course Title: CONCEPTS IN ORGANIC CHEMISTRY **Course Code : P19CH102**													
Mapping	**PO 1**	**PO 2**	**PO 3**	**PO 4**	**PO 5**	**PO 6**	**PO 7**	**PO 8**	**PO 9**	**PSO 1**	**PSO 2**	**PSO 3**	**PS0 4**
CO1	H	H	M	L	M	-	M	M	L	H	-	L	M
CO2	H	H	M	M	L	-	L	-	-	H	M	-	-
CO3	H	H	H	M	M	-	M	L	L	H	L	L	L
CO4	H	H	M	M	L	-	H	L	L	H	M	-	-
CO5	H	H	M	L	M	-	L	M	L	H	-	L	M
CO6	H	H	M	H	M	M	L	-	-	H	-	M	-

5.Course Assessment Methods

Direct

1. Continuous Assessment Test (Model Exams) I,II
2. Open book test; Cooperative learning report, Assignment; Journal paper review, Group Presentation, Project report, Poster preparation, Proto-type or Product Demonstration etc. (as applicable)
3. End Semester Practical Examination

Indirect

1. Course-end survey

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Core Course: III CHEMICAL KINETICS AND QUANTUM MECHANICS

SEMESTER : I **CODE : P19CH103**
CREDITS : 6 **TOTAL HOURS : 90**
Hours / Week:6

1.Course Outcomes

After the successful completion of this course the students will be able to

S.No.	Course Outcomes	Level	Unit
1	Correlate the kinetic properties with thermodynamic properties	K5	I
2	Deduce the rate equation from mechanistic data	K5	I
3	Solve problems by applying the principles of Kinetics and Quantum Mechanics	K5	III
4	Predict the hybridization schemes in molecules through Quantum mechanical approach of MO and VB theories	K5	IV
5	Deduce Wave functions and Energy of simple systems using Approximation methods	K5	IV
6	Analyze the mechanism of heterogeneous catalysis based on the principles of adsorption	K4	V

2A. Syllabus

UNIT-I Chemical Kinetics – I 18 Hours

1.1 Theories of reaction rates and factors influencing the reaction rate: ARRT (Eyring's theory), Thermodynamic derivation of ARRT-comparison of ARRT with collision theory (A , $\Delta S^{\#}$, E_a and $\Delta H^{\#}$) – kinetic isotope effects, Marcus electron transfer theory-inner and outer electron transfer.

1.2 Theory of unimolecular reactions-Lindemann's theory – Steady State approximation-chain reactions-photochemical reaction between hydrogen and halogens (Cl_2 and Br_2) – gas phase auto-oxidations, explosions-hydrogen-oxygen reaction.

UNIT- II Chemical Kinetics – II 18 Hours

2.1 Application of ARRT to solution kinetics-effects of solvents, double sphere model, effect of ionic strength on ionic reactions – influence of pressure on reaction rates in solution-significance of volume of activation-substituent effects – Hammett and Taft equations.

2.2 Homogeneous catalysis, acid-base catalysis – types and mechanism, derivation of rate law for protolytic acid catalysis and explanation for Arrhenius and van’t Hoff intermediates, Bronsted relations- Hammett-Deyrup

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acidity function – enzyme catalysis-mechanism of single substrate reaction-Michaelis-Menton equation - Influence of pH, concentration and temperature, Line Waver plot and Eddi – Hofstee plot.

2.3 Fast reactions-study of kinetics by stopped flow technique, relaxation methods, T and P- jump methods, flash photolysis and magnetic resonance method.

UNIT- III Quantum Chemistry-I 18 Hours

3.1 Mathematical concepts for quantum mechanics – differentiation formula for uv, u/v, (u+v), sinx, cosx, and e^x only – partial differentiation – Euler's reciprocal relation, chain rule (statement only) – Integration methods.

3.2 Inadequacy of classical mechanics-wave particle dualism – deBroglie's equation – Uncertainty principle – postulates of quantum mechanics -significance of ψ and ψ^2 ; Schrodinger time independent wave equation- Eigen functions and Eigen values - Operators and their properties – linear and Hermitian, angular momentum operators- commutation relations.- orthogonalization and normalization.

3.3 Applications of wave mechanics to simple systems – Particle in a box - one and three Dimension, Rigid rotator-Harmonic oscillator - zero point energy-Hydrogen atom- shapes and nodal properties of orbitals- Bohr's correspondence principle.

UNIT- IV Quantum Chemistry – II 18 Hours

4.1 Approximation methods – Variation method-application to one dimensional box, H_2, H_2^+ and Helium atom - Perturbation method - application to one dimensional box and Helium atom- Born Oppenheimer Approximation- Hartree method and Hartree Fock Self-consistent Field method – many electron atoms- Pauli's principle and Slater determinant.

4.2 LCAO- MO treatment of hydrogen molecular ion and H_2-VB treatment of hydrogen molecule - hybridization of orbitals in BeF_2, BF_3,CH_4. Huckel pi-electron theory and its applications to ethylene, butadiene, benzene and allyl system.

UNIT- V Surface Chemistry 18 Hours

5.1 Adsorption–physisorption and chemisorptions – Langumuir, BET & Gibbs adsorption isotherms- surface area determination – Heat of adsorption, determination. Adsorption from solutions - surface films.

5.2 Surface tension – effect of electrolytes, non-electrolytes and surface active agents –micelles andreverse micelles. Solublisation, micro emulsions

5.3 Heterogeneous catalysis – semiconductor catalysis, n-and p-type surfaces – kinetics of surface reactions involving adsorbed species – Langmuir - Hinshelwood mechanism. Langmuir – Rideal mechanism and Rideal - Eley mechanisms.

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2B.Topics for Self-Study:

S.No	TOPICS	Web Links
1	**UNIT-I (CHEMICAL KINETICS – I)** chain reactions	https://www.pdfdrive.com/chemical-kinetics-e188163536.html
2	**UNIT-II (CHEMICAL KINETICS – II)** Fast reactions – Shock Tube method	https://www.pdfdrive.com/chemical-kinetics-e188163536.html
3	**UNIT- III (QUANTUM CHEMISTRY-I)** Quantum Tunneling of Electrons	https://ocw.mit.edu/courses/chemical-engineering/10-626-electrochemical-energy-systems-spring-2014/study-materials/MIT10_626S14_Lec20.pdf
4	**UNIT- IV (QUANTUM CHEMISTRY-II)** Harmonic Oscillator: First Order Perturbation	https://physicspages.com/pdf/Griffiths%20QM/Griffiths%20Problems%2006.02.pdf
5	**UNIT- V (SURFACE CHEMISTRY)** Calculation of surface tension - Parachor method - Effect of temperature on surface tension	https://pdfs.semanticscholar.org/34e8/e28e30c040e35e022952dff3201c53fb3248.pdf

2C.Text Book(s):

1. Philip Mathews, “Advanced Physical Chemistry”, Foundation Books, New Delhi, 2003. **(Unit I-V)**
2. A.K.Chandra, “Introductory Quantum Chemistry”, Tata McGraw-Hill, New Delhi, 2017. **(Unit- III, IV)**
3. B.R. Puri, L.R.Sharma and M.S. Pathania, “Principles of Physical Chemistry”, Vishal Publishing Co., Jalandar, 2017. **(Unit-II, III, IV, V)**

2D.Reference Books:

1. Peter Atkins and Julio de Paula, “Physical Chemistry” Oxford University Press, 2018.
2. K.J. Laidler, “Chemical Kinetics”, Tata McGraw-Hill, New Delhi, 2003.
3. A.A. Frost and R.G. Pearson, “Kinetics and Mechanisms”, John Wiley & Sons, New York, 1961.

4. I. Amdur and G.G. Hammes, “Chemical Kinetics – Principles and Selected Topics”, McGraw Hill, New York, 1966.
5. J.I. Steinfeld, J.S. Francisco and W.L.Hase, “Chemical Kinetics and Dynamics”, Prentice Hall, New Jersey, 1999.
6. Horia Metiu, “Physical Chemistry-Kinetics”, Taylor and Francis, New York, 2006.
7. R.K.Dave, “Chemical Kinetics”, Campus Books, 2000.
8. D.A. Mcquarrie, “Quantum Chemistry”, University Science Books, 2016.
9. I.N.Levine, “Quantum Chemistry”, Prentice Hall, 2016.
10. R.K. Prasad, “Quantum Chemistry”, New Age international (P) Ltd., New Delhi, 2010.
11. B.K. Sen, “Quantum Chemistry”, Tata McGraw-Hill, New Delhi, 1992.
12. Thomas Engel and Philip Reid, “Physical Chemistry”, Pearson Education, New Delhi, 2013.

3.Specific Learning Outcomes (SLO)

Unit/Section	**Course Content**	**Learning Outcomes**	**Blooms Taxonomic levels of Transaction**
I	**Chemical Kinetics – I**		
1.1	Theories of reaction rates and factors influencing the reaction rate: ARRT (Eyring’s theory),Thermodynamic derivation of ARRT-comparison of ARRT with collision theory	Compare the collision theory and ARRT	K4
		Derive the Erying’s Equation	K4
		Identify the factors influencing the reaction rate.	K3
	Kinetic isotope effects	Predict the major product formed during a reaction	K5
		Evaluate the mechanisms using the magnitude of kinetic isotopic substitution	K5
		Categorize the secondary KIE depending upon the site of Isotopic substitution.	K4
	Marcus electron transfer theory-inner and outer electron transfer	Apply the Marcus electron transfer theory for different	

		systems.	K3
		Distinguish outer and inner electron theory.	K4
1.2	Theory of unimolecular reactions - Lindemann’s theory – Steady State approximation	Analyze the mechanism for unimolecular reactions	K4
		Apply the Steady State Approximation	K3
	Chain reactions-photochemical reaction between hydrogen and halogens (Cl_2 and Br_2)	Outline the mechanism of the photochemical reaction between Hydrogen and halogens	K3
		Apply the steady state approximation to photochemical reaction between Hydrogen and halogens	K3
	Gas phase auto-oxidations, explosions-hydrogen-oxygen reaction.	Determine the reaction rate for gas phase auto-oxidation	K3
		Explain how branching chain reactions can lead to explosion.	K2
II	**Chemical Kinetics – II**		
	Application of ARRT to solution kinetics: Effects of solvents, double sphere model	Analyze the effect of solvents on reaction rate	K4
		Explain the effect of dielectric constant using double sphere model.	K2
		Predict the kinetic model for unknown system.	K5

2.1	Effect of ionic strength on ionic reactions	Explain the kinetic salt effect	K5
		Examine the influence of ionic strength on the rate of reaction	K4
	Influence of pressure on reaction rates in solution- Significance of volume of activation	Relate pressure with the rate of a reaction.	K2
		Derive volume of activation from the pressure dependence nature of rate constant.	K4
	Substituent effects – Hammett and Taft equations.	Predict the effect of substituent on the acidity of an aromatic carboxylic acid.	K5
		Justify the pKa for the phenols using the appropriate substituent constants.	K5
		Recommend a mechanism for a given reaction by determining the reaction constant.	K5
		Predict the structure of the transition state for a given reaction.	K5
		Determine the reaction constants for the effects of substituent X and Y using the appropriate substituent constants.	K5
		Apply Taft equation in predicting the reaction mechanisms.	K3

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		Develop quantitative structure –activity relationships for organic compounds using Taft Equation.	K3
2.2	Homogeneous catalysis, acid-base catalysis – types and mechanism	Explain the kinetics of acid-base catalyzed reactions.	K5
		Determine the order of a given acid-base catalyzed reaction.	K5
	Derivation of rate law for protolytic acid catalysis and explanation for Arrhenius and van't Hoff intermediates	Deduce the rate expression for protolytic acid catalysis	K4
		Compare the formation and stability of Arrhenius and van't Hoff intermediates.	K4
	Bronsted relations - Hammett-Deyrup acidity function	Deduce Bronsted relationship for acid/ base catalysis	K4
		Assess the acidity of strong acids using Hammett acidity function.	K5
		Correlate between chemical reactivity and the Hammett Acidity function	K4
	Enzyme catalysis-mechanism of single substrate reaction-Michaelis-Menton equation - Influence of pH, concentrationand temperature	Explain the mechanism of enzyme catalyzed reactions	K5
		Deduce Michaelis-Menton equation.	K4
		Illustrate the pH and Temperature dependence of enzyme catalyzed reactions	K4
	Line weaver plot and Eddi –	Explain the kinetics of reactions using Line weaver	K5

	Hofstee plot.	plot	
		Analyze the mechanism of enzyme kinetics using Eddi – Hofstee plot.	K4
		Predict the optimal conditions for enzyme catalysis.	K5
2.3	Fast reactions-study of kinetics by stopped flow technique, Relaxation methods, T and P-jump methods Flash photolysis and Magnetic resonance method	Explain the kinetics of fast reactions by: Stopped flow technique, Relaxation methods, Flash photolysis Magnetic resonance method	K3
III	**Quantum Chemistry-I**		
3.1	Mathematical concepts for quantum mechanics – differentiation formula for uv, u/v, (u+v), sinx, cosx, and e^x only – partial differentiation – Euler's reciprocal relation, chain rule (statement only) – Integration methods.	Apply the differentiation formulae for quantum mechanics.	K3
		Apply the Integration methods in Quantum mechanical derivations.	K3
	Inadequacy of classical mechanics	Explain the limitations of classical mechanics	K2
		Explain the need for Quantum mechanics.	K2
	Wave-Particle Dualism – de Broglie's equation – Uncertainty principle.	Find out the de Broglie's wave length of a moving object.	K3
		Solve problems on Uncertainty principle	K3
	Postulates of quantum mechanics -significance of ψ and ψ^2	Summarize the postulates of Quantum mechanics	K2
		Explain the significance of ψ	K2

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3.2		and ψ^2	
		Evaluate the well-behaved nature of selected parameters.	K5
	Schrodinger time independent wave equation-Eigen functionsand Eigen values	Deduce the Schrodinger time independent wave equation	K2
		Define Eigen functions and Eigen values	K1
	Operators and their properties – linear and Hermitian, angular momentum operators-commutation relations	Classify the quantum mechanical operators	K2
		Explain the properties of different operators	K4
		Deduce Commutation relations for operators	
		Aapply the principles of operators in unknown systems.	K3
		Describe the dynamic properties of microscopic bodies using the principles of Quantum mechanics	K2
	Orthogonalization and Normalization.	Evaluate the wave functions of different systems using the conditions of Orthogonalization and Normalization.	K5
	Applications of wave mechanics to simple systems: Particle in a one Dimensional box	Deduce the Schrodinger wave equation for Particle in a one Dimensional box and solve it for ψ and Energy.	K4

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3.3	Particle in a 3- Dimensional box Rigid rotator Simple Harmonic oscillator - zero point energy	Deduce the Schrodinger wave equation for Particle in a 3- Dimensional box and solve it for ψ and Energy.	K4
		Construct the Schrodinger wave equation for Rigid rotator and solve it for ψ and Energy.	K3
		Deduce the Schrodinger wave equation for a Simple Harmonic oscillator and solve it for ψ and Energy.	K4
	Hydrogen atom- shapes and nodal properties of orbitals - Bohr's correspondence principle.	Prove Bohr's correspondence principle.	K3
IV	**Quantum Chemistry –II**		
4.1	Approximation methods – Variation method-application to one dimensional box, H_2, H_2^+ and Helium atom	Apply the variation methodto Hydrogen and Hydrogenlike atoms.	K3
	Perturbation method - application to Helium atom	Apply the Perturbation method to Helium atom	K3
	Born Oppenheimer Approximation	Outline the uses and failures of Born Oppenheimer Approximation	K2
	Hartree method and Hartree Fock Self-consistent Field method – many electron atoms	Outline the Hartree-Fock SCF theory of polyatomic molecules.	K3
		Apply the HFSCF method to Simple systems with more than one electrons such as Li, Be,etc.	K3
	Pauli's principle and Slater determinant.	Write the Slater determinats for a given electronic	K3

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		configuration.	
		Predict the solutions of the Schrodinger wave equation for poly electron systems using the Pauli’s exclusion principle and appropriate Slater determinant.	K5
4.2	LCAO- MO treatment of hydrogen molecular ion and H_2	Deduce the normalized wave function for the BMO and ABMO using the LCAO for the wave function for H_2^+ ion	K4
	Hybridization of orbitals in BeF_2, BF_3 andCH_4.	Construct the wave functions for sp, sp^2, sp^3 hybrid orbitals.	K3
	Huckel pi-electron theory and its applications to Ethylene, Butadiene, Benzene and Allyl system.	Construct and solve Huckel secular determinantal equation for Ethylene, Butadiene and Benzene, using HMO theory.	K3
V	**Unit – 5: Surface Chemistry**		
5.1	Adsorption–physisorption and chemisorptions	Differentiate Physisorption and Chemisorption	K3
		Summarize the factors influencing adsorption of agas on a solid.	K2
		Calculate the volume of a gas that is adsorbed by an adsorbent.	K3
	Langumuir, BET & Gibbs adsorption isotherms - Surfacearea determination	Deduce the adsorption isotherms	K4
		Calculate the surface area of the adsorbent	K3
	Heat of adsorption determination. Adsorption from solutions -	Deduce an expression which shows the variation of	K4

	surface films.	surface film pressure with film area.	
5.2	Surface tension – effect of electrolytes, non-electrolytes	Explain the variation of surface tension of a solvent by the addition of a solute.	K2
	Surface active agents –micelles and reverse micelles.	Show how the physical properties of solutions of surfactants such as molar conductance, surface tension, osmotic pressure change at critical micelle concentration.	K2
	Solublisation, micro emulsions	Discuss the methods used in finding the type of an emulsion.	K2
5.3	Heterogeneous catalysis – semiconductor catalysis, n-and p-type surfaces	Explain the transfer of reaction from the gas phase to the surface of a semiconductor result in facilitation of the reaction.	K4
		Analyze the mechanism of the action of semiconductor.	K4
		Explain the role of the catalyst in the transformation of molecules into surface radicals.	K3
	Kinetics of surface reactions involving adsorbed species – Langmuir - Hinshelwood mechanism. Langmuir – Rideal mechanism and Rideal - Eley mechanisms.	Describe the Langmuir – Hinshelwood mechanism for chemical reactions catalyzed on surfaces.	K2
		Discuss the mechanism of photocatalytic reactions.	K2

4.Mapping (CO, PO, PSO)

L-Low **M-Moderate** **H- High**

Course Title: CHEMICAL KINETICS AND QUANTUM MECHANICS Course Code : P19CH103													
	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PSO1**	**PSO2**	**PSO3**	**PSO4**
CO1	H	M	H	H	H-	-	M	M	-	H	H	H	-
CO2	H	H	M	H	H	-	H	M	-	H	H	H	L
CO3	H	H	M	H	-	-	M		-	H	M	H	H
CO4	H	M	-	-	-	-	M		-	H	M	H	M
CO5	H	L	-	-	-	-	M		-	H	M	H	H
CO6	H	L	H	M	H	-	H	M	-	H	H	H	-

5.Course Assessment Methods

Direct:

1. Continuous Assessment Test (Model Exams) I,II
2. Open book test; Cooperative learning report, Assignment; Journal paper review, Group Presentation, Project report, Poster preparation, Proto-type or Product Demonstration etc. (as applicable)
3. End Semester Practical Examination

Indirect

1. Course-end survey

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Core Practical : I

INORGANIC QUANTITATIVE ESTIMATIONS AND COMPLEX PREPARATION (Lab cum Theory)

Semester : I **Code : P19CH1P1**
Credits : 3 **Total Hrs : 90**
Hours /week:6

1.Course Outcomes:

At the end of this course, the student will be able to

S.No.	Course Outcomes	Level
1	Formulate a methodology for separation of metal ions from mixtures	K6
2	Estimate metal ions present in a mixture	K5
3	Propose scheme for synthesizing inorganic complexes	K6
4	Interpret UV-Visible spectra of the given inorganic complexes	K5
5	Predict the nature of bonding in coordination compounds using UV-Vis spectra	K5
6	Choose an appropriate method for estimating metal ions in industrial effluents	K5

2A. Syllabus

1. TITRIMETRY AND GRAVIMETRY:

Only mixture(s) of solutions should be given for estimation
(i) Cu(V) and Ni (G) (ii)Cu(V) and Zn (G)
(iii)Fe(V) and Ni (G) (iv)Zn(V) and Cu (G)
(v)Fe(V) and Zn (G)

2. PREPARATION OF THE FOLLOWING COMPLEXES:

Tetraamminecopper(II)sulphate
Potassium trioxalatochromate (III)
Potassium trioxalatoaluminate (III)
Tristhioureacopper (I) chloride
Tristhioureacopper (II)sulphate

3. UV – VISIBLE SPECTRAL STUDIES:

Recording UV-visible spectrum of five coordination complexes and interpretation of the spectra (demonstration only).

2B.Text Books:

1. Vogel’s, Text Book of Inorganic Qualitative Analysis, 4th Edition, ELBS, 1974
2. Vogel’s, Quantitative Chemical Analysis, 6th Edition, Pearson Education, 2009

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2C.Reference Books:

1. Jeffery G. Bassett.J, Mendhan, R. C. Vogel's "Textbook of Qualitative Chemical Analysis" 5th Edition, ELBS, 1989.

3.Specific Learning Outcomes (SLO)

Course Content	**Learning Outcomes**	**Blooms** Taxonomic levels of transaction
1. Titrimetry and Gravimetry Only mixture(s) of solutions should be given for estimation – (i) Cu (V) and Ni (G), (ii) Cu (V) and Zn (G) (iii) Fe (V) and Ni (G) (iv) Zn (V) and Cu (G) and (v) Fe (V) and Zn (G)	Distinguish the primary and secondary standard solutions.	K3
	Prepare solutions of different concentration units (upto ppm level)	K3
	Develop their skills in estimating metal ions by volumetry and gravimetry.	K5
	Develop methodology to quantitatively separate metal ionin the presence of other metal ions	K5
	Estimate quantitatively the metal ion in a mixture of metal ions	K6
2. Preparation of Coordination Compounds i) Tetramminecopper(II)sulphate, ii) Potassium trioxalatochromate (III) iii) Potassium trioxalatoaluminate (III) iv) Tristhioureacopper(I)chloride v) Tristhioureacopper(I)sulphate	Distinguish the distinct features of complexes over double salts.	K2
	Apply their skills and methodology to prepare a complex with high purity.	K3
	Propose scheme for synthesizing inorganic complexes	K6
3. UV – Vis Spectral characterization (demonstration only) i) Tetrammine copper(II)sulphate,	Justify UV-Visible absorption spectra of inorganic complexes	K6
	Deduce the geometry of the complex	K4

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ii) Potassium trioxalatochromate (III) iii) Potassium trioxalatoaluminate (III) iv) Tristhioureacopper(I)chloride v) Tristhioureacopper (I)sulphate	Summarize the basic principle, instrumentation and method of sampling involved in UV-Visible spectrophotometry.	K2

4.Mapping Scheme for the PO, PSOs and COs

L-Low **M-Moderate** **H- High**

Course Title: **INORGANIC QUANTITATIVE ESTIMATIONS AND COMPLEX PREPARATION**
Course Code : P19CH1P1

Mapping	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PSO1	PSO2	PSO3	PSO4
CO1	**M**	**H**	**M**	**H**	**H**	**M**	**H**	**M**	**-**	**H**	**H**	**L**	**H**
CO2	**L**	**M**	**M**	**M**	**L**	**-**	**H**	**H**	**L**	**H**	**H**	**M**	**H**
CO3	**M**	**H**	**M**	**M**	**M**	**L**	**M**	**L**	**L**	**H**	**M**	**M**	**H**
CO4	**L**	**H**	**M**	**H**	**H**	**M**	**H**	**H**	**H**	**M**	**M**	**L**	**H**
CO5	**H**	**H**	**-**	**H**	**H**	**H**	**H**	**L**	**M**	**H**	**-**	**H**	**H**
CO6	**H**	**H**	**H**	**H**	**M**	**M**	**-**	**-**	**L**	**H**	**-**	**H**	**H**

5.Course Assessment Methods

Direct
1. Continuous Assessment 2. Model Exam 1 & 2 3. Viva -Voce 4. End Semester Examination
Indirect
1. Course-end survey

Core Practical - II ORGANIC SYNTHESIS AND SEPARATION TECHNIQUES

Semester: I **Code: P19CH1P2**
Credits: 3 **Total Hrs.: 90**
Hours/ week:6

1.Course Outcomes:

At the end of this course, the student will be able to:

CO1: Choose appropriate solvent for separation of a binary mixture of organic compounds (K5)
CO2: Test the functional groups present in organic compounds (K5)

CO3: Plan a scheme for the synthesis of organic compounds (K6)

CO4: Infer purity of synthesized compounds by determining their physical constants (K4)

CO5: Separate the organic compounds in a mixture by column chromatographic technique (K4)

CO6: Predict the completion of reaction by thin layer chromatographic technique (K5)

2A.Syllabus

EXPERIMENTS:

1. Solvent separation of the binary mixture by Pilot & Bulk Analysis.
2. Report the Melting/Boiling Points of the pure compounds.
3. Systematic Semi micro spot analysis & derivatization of Organic Compounds.

Preparations, Recrystallization & determination of Melting points of the two products:

1. Cinnamic acid from Benzaldehyde.
2. p-nitroacetanilide from Aniline.
3. Alpha & Beta – D- Glucose penta acetate from the given quantity of Glucose.
4. Aspirin from the given quantity of Methyl Salicylate.
5. 2,4-dinitrophenylhydrazones of Benzaldehyde and Ethyl methyl ketone.

- Separation of pure compounds by Column Chromatrographic Separation.
- Monitoring reaction mechanism by Thin layer Chromatography Separation.

2C.Reference Books :

1. Syed Mumtazuddin, Organic Chemistry – A Laboratory Manual, Narosa Publishing House,New Delhi, 2014.
2. Syed Mumtazuddin, Advanced Practical Chemistry, Syed Mumtazuddin,Pragati Prakashan, Meerut, 2014

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3. V K Ahluwalia & Sunita Dhingra, Advanced Experimental Organic Chemistry, Manakin Press, New Delhi, 2017.
4. Sonia Ratnani Experimental Organic Chemistry, PHI Learning Private Ltd., New Delhi, 2012

3.Specific Learning Outcomes (SLO)

Unit	Course Content	Learning Outcomes	Blooms Taxonomic levels of Transaction
1.1	Solvent separation of the binary mixture by Pilot & Bulk Analysis	Select different types of work-up like acid-base and neutral work-up	K5
		Determine the nature of organic compound present in the mixture	K5
1.2	Report the Melting/Boiling Points of the pure compounds	Deduce the purity of the prepared pure sample	K4
1.3	Systematic Semimicro spot analysis& derivatization of Organic Compounds	Analyse the given organic compound systematically and prepare a suitable derivative	K4
1.4	**Preparations, Recrystallization & determination of Melting points of the two products** 1. Cinnamic acid from benzaldehyde 2. p-nitroacetanilide from aniline 3. Alpha & beta – D-glucose penta acetate from the given quantity of glucose 4. Aspirin from the given quantity of methylsalicylate 5. 2,4-dinitrophenylhydrazones of benzaldehyde and ethyl methyl ketone	Construct scheme and develop skill of organic synthesis	K6
		Devise purification technique to obtain pure product	K4
		Deduce the purity of prepared product by melting point determination.	K4
2.1	Separation of pure compounds by	Divide the mixture into individual compound	K4

	column chromatographic Separation	Select the correct eluent system	K4
		Choose column length based on the nature of impurities.	K3
2.2	Monitoring reaction mechanism by thin layer chromatography separation	Predict the progress of reaction by TLC.	K5
		Select right eluent system to separate the mixture.	K4

4.Mapping Scheme for the PO, PSOs and Cos

L-Low **M-Moderate** **H- High**

Course Title: ORGANIC SYNTHESIS AND SEPARATION TECHNIQUES
Course Code: P19CH1P2

Mapping	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PSO1	PSO2	PSO3	PSO4
CO1	H	H	H	M	M	-	M	H	L	M	M	L	M
CO2	H	H	H	H	H	-	M	H	L	H	M	M	H
CO3	H	H	H	H	H	-	H	M	H	H	H	H	H
CO4	H	L	H	L	M	L	L	M	L	L	L	L	L
CO5	H	H	M	H	H	-	H	M	H	H	M	L	H
CO6	H	H	M	H	H	-	H	M	H	H	M	L	H

5.Course Assessment Methods

Direct

1. Continuous Internal Assessment
2. Model Exam 1 & 2
3. Viva -Voce
4. End Semester Examination

Indirect

1. Course-end survey

PRACTICAL PREPARATORY COURSE-I

(For Organic and Inorganic Practical)

SEMESTER : I **COURSE CODES: P19CH1P1& P19CH1P2** **TOTAL HOURS: 30**

COURSE OBJECTIVES:

- To appreciate the idea behind laboratory experiments in P19CH1P1& P19CH1P2.
- To understand the concepts behind qualitative and quantitative techniques in Organic and Inorganic Practical.

UNIT – I PRINCIPLES IN SEPARATION OF BINARY MIXTURE

Solvent polarity – Miscibility of organic compounds in ether / water – principles of solvent extraction- partitioning of solutes – regeneration of organic components and purification and Recrystallisation. Basic steps involved in bulk separation.

UNIT – II PRINCIPLES & PROTOCOLS FOR PREPARATION

Mechanistic details of preparations performed and the conditions to be maintained- green aspects of the preparation – Simple steps for recycling products – Techniques of Recrystallisation.

UNIT - III

BASIC PRINCIPLES OF INORGANIC VOLUMETRIC AND GRAVIMETRIC ANALYSIS

Recollection of Concentration terms- Preparation of primary and secondary standards-Types of titrations- Indicators (Redox and internal)- stoichiometry of gravimetric reactions– Common errors in volumetry and gravimetry – methods of reducing errors. Difference between double salts and complexes – protocols and conditions in preparation of complexes- spectral identification of d-d transitions in the complexes prepared (demonstration)

UNIT- IV CHROMATOGRAPHIC METHODS

Basic principles of adsorption and partition chromatography – Cautions in preparation and development of chromatograms (both paper and TLC) – Polarity of solvents and elution –Different spotting reagents for identification of organic compounds.

TEXT BOOKS:

1. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, 3rd Edition, The National Publishing Company, Chennai -1, 2004.
2. Gnanaprakasan N.S. & G. Ramamurthy, Organic Chemistry Lab Manual, S. Viswanathan Pvt. Ltd, Chennai -31, 2007.

REFERENCES:

1. R.A. Day & A.L. Underwood, Quantitative Analysis, 6th Edition, PHI Learning Pvt. Ltd., New Delhi, 2009.
2. Arun Sethi, Systematic Experiments in Chemistry, New Age International Pvt. Ltd, New Delhi. 2009.

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COMPONENTS FOR EVALUATION

TEST - 1 : **Max marks: 30 (Part A - 2 X 10, Part B - 2x5)**

TEST – 2 : **Max marks: 30 (Part A - 2 X 10, Part B - 2x5)**

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Core Course -IV COORDINATION AND ORGANOALLIC CHEMISTRY

Semester : II **Code : P19CH204**
Credits : 6 **Total Hrs : 90**
Hours/week:6

1.Course Outcomes:

After the successful completion of this course, the students will be able to :

S.No	Topic	Level	Unit
1.	Evaluate Crystal Field Stabilization Energy of Coordination compounds based on splitting pattern derived from CFT and MOT	K5	I
2.	Explain reaction-mechanism and stability constant of coordination compounds	K4	II
3.	Categorize various photochemical reactions of coordination compounds	K4	III
4.	Explain structure, bonding and stability of organometallic compounds	K5	IV
5.	Predict the products obtained from different reactions of organometallic compounds	K5	V
6.	Summarize the potential applications of organometallic compounds as industrial Catalysts	K5	V

2A. Syllabus

UNIT–I CO-ORDINATION CHEMISTRY 18 Hours

1.1 Nomenclature of mono and polynuclear complexes. Crystal Field theory –Splitting of d orbitals in octahedral symmetry – CFSE - strong field and weak field splitting – calculation of CFSE for dn system. Factors affecting the magnitude of splitting (10Dq). Splitting in tetrahedral symmetry – only weak field splitting – reasons. Tetragonal symmetry – differences between tetrahedral and tetragonal symmetry.

1.2 Jorgensen's relation, Spectrochemical series, Nephelauxetic effect, Jahn–Teller theorem and J-T distortion.

1.3 M.O theory of Octahedral complexes(sigma and pi bonding) , M.O theory of tetrahedral and square planar complexes.

UNIT–II Kinetics and mechanisms of reactions in solutions 18 Hours

2.1 Labile and inert complexes, ligand displacement reactions – Acid hydrolysis, base hydrolysis SN1CB mechanism and anation reactions in octahedral and square planar complexes–Transeffect-theories and applications. Electron transfer (ET) reactions – electron exchange reactions-complementary and non – complementary types. Types – Inner sphere and Outer sphere processes – Applications of ET reactions in inorganic complexes. Isomerization and racemization reactions of complexes – Reactions of the coordinating ligands.

2.2 Stability of Coordination compounds: Stability constants - stepwise and overall formation constants – Factors affecting stability constant-Irwing William series- Spectrometric and Jobs methods of determining stability constant.

UNIT–III INORGANIC PHOTOCHEMISTRY 18 Hours

3.1 Laws of photochemistry- photophysical processes- Jablonski diagram- Fluorescence-phosphorescence- Kasha's rule- Stoke's shift- Types of electronic transitions in metal complexes –Photochemical transitions in metal complexes

3.2 Photo-substitution, photo-oxidation, photo- reduction, photo-aquation, photo-isomerization

and Unimolecular charge-transfer

3.3 Photochemistry of Cobalt(III) complexes, Ligand field photochemistry of chromium(III) complexes, Adamson's rules, Photochemistry of ruthenium –polypyridine complexes, Photochemistry of organometallic compounds,Chemical actinometers- Reinecke' salt, Uranyl oxalate and Potassium ferrioxalate actinometer.

UNIT-IV ORGANOMETALLIC CHEMISTRY 18Hours

4.1 General introduction of organometallic complexes (a) 18-electron compounds (b) 16-electron square planar compounds- Electron count preference- 18 electron rule- (a) neutral-ligand method (b) Donor –pair method. Hapticity - Isolobal Analogy and its limitations.

4.2 Structure and bonding of organometallic complexes with various types of ligands such as carbon monoxide (Metal Carbonyls), phosphines, Hydrides and dihydrogen complexes. η1-alkyl,-alkenyl,-alkynyl and –aryl ligands. η2 –alkene (metal olefins Zeise’s Salt),–alkyne ligands, non conjugated diene and polyene ligands. Dinitrogen and nitrogen monoxide (metal nitrosyls). The allyl ligand- η1 and η3 allyl complexes. Butadiene, cyclobutadiene , cyclooctatetraene, benzene and other arenes

4.3 Metallocenes-(a) synthesis and reactivity of cyclopentadienyl compounds (Ferrocene) –(b) bonding in bis (cyclopentadienyl) metal complexes M.O. theory, (c) fluxional behaviour of metallocenes and (d) bent metallocene complexes

UNIT–V CATALYSIS IN ORGANOMETALLICS 15 Hours

5.1. Catalyst-types of catalyst-catalytic steps-(a)Ligand co-ordination and dissociation-(b) insertion(1,1-migratory insertion reactions) and elimination - (1,2 –insertions and β-hydride elimination) (c) nucleophilic attack on co-ordinated ligands (d) oxidation and reduction , (e) oxidative addition and reductive elimination.

5.2. Hydrogenation of olefins (Wilkinson's Catalyst)- hydroformylation (Oxo process)- Oxidation of Olefins (Wacker process)-Acetic acid synthesis(Monsanto process)- Polymerisation (Ziegler Natta Catalyst) of alkenes- Oligomerisation-Metathesis-σ bond metathesis, alkene metathesis and Ene-yne metathesis- Fischer -Tropsch Synthesis.

2B.Topics for Self-Study:

S.No	Topic	Weblink
1.	Applications of Coordination Compounds in Biological System	https://www.ias.ac.in/article/fulltext/reso/016/12/1273-1283 https://www.youtube.com/watch?v=c2UmZOwy2UY
2.	Transition Metal Allyl and Enyl Complexes	https://www.digimat.in/nptel/courses/video/104101100/L01.html
3.	Biomedical Applications of Photochemistry	http://hub.hku.hk/handle/10722/129257 http://hub.hku.hk/bitstream/10722/129257/1/content.pdf
4.	NMR Spectroscopy of Organometallic compounds	https://www.researchgate.net/publication/261531508_NMR_in_Organometallic_Chemistry_Von_Paul_S_Pregosin https://www.youtube.com/watch?v=0GFitxSn-T0 https://sci-hub.se/10.1016/S0065-3055(08)60118-5

2C.Text Books

1. James E. Huheey, Ellen A Keiter and Richard L. Keiter, "Inorganic Chemistry: Principles of Structure and Reactivity", Pearson Education, India, 2014. **(Unit I, II, IV, V)**
2. S. Arunachalam, "Photochemistry of Inorganic compounds", 2001 **(Unit- III)**

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2D.Reference Books

1. D.F. Shriver and P.W.Atkins, “Inorganic Chemistry”, Oxford, New Delhi, 2006.
2. Keith F. Purcell and John C. Kotz, “Inorganic Chemistry”, Saundera Goldern Sunburst Series, W.B. Saunders Company, Philadelphia, 2010.
3. J.D. Lee, “A New Concise Inorganic Chemistry”, Oxford University Press, New Delhi,2008.
4. F. Albert Cotton, Geoffrey Wilkinson and Carlos A. Murillo, “Advanced Inorganic Chemistry” John Wiley & Sons, Singapore, 2007.
5. Raymond Chang, “Chemistry” Tata McGraw Hill, New Delhi, 2008.
6. Alan G. Sharp, “Inorganic Chemistry”, Addison – Weseley, New York, 1999.
7. Gary L. Miessler, Donald A. Tarr, “Inorganic Chemistry”, Pearson Education, New Delhi, 2008.
8. A. W. Adamson, “Inorganic Photochemistry”, John Wiley & sons, New York, 2000
9. B.R. Puri, L.R. Sharma and K.C. Kalia “Principles of Inorganic Chemistry” – Vishal Publishing Co., Jalandhar, 2017.

3.Specific Learning Outcomes (SLO)

Unit	Course Content	Learning outcomes	Blooms Taxonomic levels of Transaction
	Unit-I		
1.1	Nomenclature of mono and polynuclear complexes.	Identify the structure of the mono and polynuclear complexes.	K2
	Crystal Field theory –Splittingof d orbitals in octahedral symmetry	Deduct the splitting of d –orbitals in octahedral complexes.	K5

	CFSE - strong field and weak field splitting – calculation of CFSE for d^n system. Factors affecting the magnitude of splitting (10Dq)	Evaluate Crystal Field Stabilization Energy for given complexes.	K5
		Recall the factors affecting the magnitude of splitting.	K1
	Splitting in tetrahedral symmetry – only weak field splitting – reasons.	Determine the splitting of d – orbitals in tetrahedral complexes.	K3
		List out the reasons for weak field splitting.	K3
	Tetragonal symmetry – differences between tetrahedral and tetragonal symmetry.	Distinguish tetrahedral and tetragonal symmetry with an example.	K4
1.2	Jorgensen’s relation, Spectrochemical series, Nephelauxetic effect,	Recall Jorgensen’s relation, Spectrochemical series and Nephelauxetic effect.	K1
	Jahn–Teller theorem and J-T distortion.	Examine the complex for distortion based on Jahn–Teller theorem.	K4
1.3	M.O theory of Octahedral complexes(sigma and pi bonding)	Construct M.O diagram for octahedral complexes.	K3
	M.O theory of tetrahedral and square planar complexes.	Construct the M.O diagram for tetrahedral and square planar complexes.	K3
	Unit-II		
2.1	Labile and inert complexes, ligand displacement reactions – Acid hydrolysis, base hydrolysis SN1CB mechanism	Classify Labile and inert complexes with examples.	K2
		Compare Acid hydrolysis, and base hydrolysis of complexes using SN_1CB mechanism	K4
	Anation reactions in octahedral and square planar complexes	Compare anation reactions in octahedral and square planar complexes	K4
	Trans effect- theories and applications. Electron transfer (ET) reactions – electron	Predict the product of the reactions based on Trans effect.	K3

	exchange reactions- complementary and non – complementary types	Differentiate complementary and non – complementary reactions.	K3
	Types – Inner sphere and Outer sphere processes	Explain the Inner sphere and Outer sphere processes in the given complex.	K4
	Applications of ET reactions in inorganic complexes. Isomerisation and racemisation reactions of complexes – Reactions of the coordinating ligands.	Categorize isomerisation and racemisation reactions in complexes based on ET .	K4
2.2	Stability constants - stepwise and overall formation constants	Outline the importance of Stability constant	K2
	Factors affecting stability constant-Irwing William series-	List out the factors affecting stability constant	K1
	Spectrometric and Jobs methods of determining stability constant.	Find stability constant based on Spectrometric and Jobs methods	K1
	Unit-III		
3.1	Laws of photochemistry- photophysical processes- Jablonski diagram-	Define Laws of photochemistry.	K1
		Explain photophysical processes using Jablonski diagram	K4
	Fluorescence- phosphorescence- Kasha's rule- Stoke's shift-	Relate Kasha's rule with fluorescence and phosphorescence	K3
	Types of electronic transitions in metal complexes	Explain CTTM, CTTL and CTTS in metal complexes.	K4
	Photochemical transitions in metal complexes Photo-substitution, photo-oxidation, photo- reduction, photo-aquation, photo-isomerization and Unimolecular charge-transfer Photochemistry of Cobalt(III) complexes	Categorize the given photochemical reactions with examples.	K4

	Ligand field photochemistry of chromium(III) complexes Adamson's rules	Apply Adamsons rule to photo-aquation reaction of chromium(III) complexes	K3
	Photochemistry of ruthenium – polypyridine complexes	Explain the Photochemistry of ruthenium –polypyridine complexes	K2
	Photochemistry of organometallic compounds	Explain the types of photochemical reactions in organometallic compounds	K2
	Chemical actinometers- Reinecke' salt, Uranyl oxalate and Potassium ferrioxalate actinometer.	Summarize the importance of actinometer.	K2
		Construct actinometers	K3
	Unit-IV		
4.1	General introduction of organometallic complexes (a) 18-electron compounds (b) 16-electron square planar compounds-	Relate 18- electron rule and 16-electron rule to octahedral and square planar compounds respectively.	K3
	Electron count preference- 18 electron rule- (a) neutral-ligand method (b) Donor –pair method.	Examine the stability of organometallic complexes based on 18- electron rule.	K3
	Hapticity **-** Isolobal Analogy and its limitations	Recall Hapticity concept.	K1
		Identify isolobal fragments	K3
4.2	Structure and bonding of organometallic complexes with ligands such as carbonmonoxide (Metal Carbonyls), phosphines, Hydrides and dihydrogen	Identify terminal and bridging carbonyls using IR stretching frequency	K3
		Compare the basicity of the various substituted phosphines.	K5
	Structure and bonding of organometallic complexes with ligands such as η^1-alkyl,-alkenyl,-alkynyl and –aryl ligands.	Explain the mode of bonding in organometallic complexes along with hapticity concept.	K5

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	Structure and bonding of organometallic complexes with ligands such as η^{2} –alkene (metal olefins Zeise's Salt),–alkyne ligands, non conjugated diene and polyene ligands.	Examine the mode of bonding in conjugated and nonconjugated systems	K3
	Structure and bonding of organometallic complexes with ligands such as Dinitrogen and nitrogen monoxide (metal nitrosyls)	Differentiate bent and linear nitrosyl complexes.	K2
		Identify the variation of bond length in dinitrogen complex	K3
	Structure and bonding of organometallic complexes with ligands such as The allyl ligand-η^{1} and η^{3} allyl complexes.	Explain the structure of organometallic complexes along with hapticity concept.	K5
	Structure and bonding of organometallic complexes with ligands such as Butadiene, cyclobutadiene , cyclooctatetraene, benzene and other arenes	Identify δ bonding interaction in the organometallic complexes with ligands such as Butadiene.	K3
4.3	Metallocenes- synthesis and reactivity of cyclopentadienyl compounds (Ferrocene)	Recall the synthesis and reactivity of ferrocene.	K1
	Bonding in bis (cyclopentadienyl) metal complexes M.O. theory,	Construct M.O diagram of ferrocene.	K3
	Fluxional behaviour of metallocenes and bent metallocene complexes	Illustrate Fluxional behaviour of metallocenes and bent metallocene complexes	K2
	Unit-V		
5.1	Catalyst-types of catalyst-catalytic steps-(a)Ligand co-ordination and dissociation-(b) insertion(1,1-migratory insertion reactions,1,2 –insertions)	Infer the basic catalytic steps.	K2
		Classify the types of catalyst	K4
		Identify the nature of ligand insertions	K1

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	Elimination - β-hydride elimination) nucleophilic attack on co-ordinated ligands	Analyze the product of the particular reaction and find the nature of elimination.	K4
	Oxidation and reduction , oxidative addition andreductive elimination.	Predict the product of the reaction based on oxidative addition and reductive elimination	K5
5.2	Hydrogenation of olefins (Wilkinson's Catalyst)-hydroformylation (Oxo process)	Construct Tolman catalytic loops for Wilkinsons catalyst.	K3
		Explain the various steps involved in Oxo process.	K5
	Oxidation of Olefins (Wacker process)-Acetic acid synthesis(Monsanto process)	Prioritize the reactions involved in Wacker process.	K5
		Explain the various reactions involved in Monsanto process.	K5
	Polymerisation (Ziegler Natta Catalyst) of alkenes-Oligomerisation	Explain Ziegler Natta Polymerisation and Oligomerisation	K5
	Metathesis-σbond metathesis,alkene metathesis and Ene-yne metathesis	Compare the metathesis in σ bond, alkene and Ene-yne metathesis with an example.	K5
	Fischer-Tropsch Synthesis.	Evaluate the mechanism of Fischer –Tropsch process.	K4

4.Mapping Scheme for the PO, PSOs and COs

L-Low M-Moderate H- High

Course Title: COORDINATION AND ORGANOALLIC CHEMISTRY
Course Code : P19CH204

Mapping	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PSO1	PSO2	PSO3	PSO4
CO1	H	M	M	-	L	M	L	M	-	M	-	L	-
CO2	M	L	L	M	L	M	-	H	-	H	M	-	-
CO3	M	L	H	-	-	M	L	M	-	M	-	H	-
CO4	M	H	L	M	L	-	-	M	-	H	-	L	-
CO5	M	H	L	-	L	M	L	L	-	M	M	L	-
CO6	M	H	L	-	L	L	-	M	-	L	H	L	-

5.Course Assessment Methods

Direct

1. Continuous Assessment Test (Model Exams) I,II
2. Open book test; Cooperative learning report, Assignment; Journal paper review, Group Presentation, Project report, Poster preparation, Proto-type or Product Demonstration etc. (as applicable)
3. End Semester Practical Examination

Xxxx- Revised content

Indirect

1. Course-end survey

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Core Course – V

REACTIONS AND MECHANISMS IN ORGANIC CHEMISTRY

Semester : II **Code : P19CH205**
Credits : 6 **Total Hours :90**

1. Course Outcomes

After the successful completion of this course the students will be able to

S.No.	Course Outcomes	Level	Unit
1	Apply the molecular orbital symmetry to predict the feasibility of pericyclic reactions at different conditions	K3	I
2	Classify different types of Photochemical reactions and their mechanism	K4	II
3	Illustrate organic reaction mechanism based on selectivity of reagent, nature of substrate-structure and reaction condition	K4	III
4	Predict the mechanism of addition reactions with respect to different functional groups and reagents	K5	IV
5	Justify the reactivity of different oxidizing and reducing agents	K5	V
6	Decide the stereochemistry of reaction products with respect to the nature of reagent and condition	K5	V

2A Syllabus

UNIT – I PERICYCLIC REACTIONS 18 Hours

Frontier Orbital Description and correlation approach of – Woodward Hofmann rules - Regiochemistry- Stereochemical aspects- Endo/Exo selection - role of secondary orbital interaction in the following:

Diels Alder Reactions (including 1,3 dipolar additions intramolecular reaction -the retro diels-alder reaction- asymmetric diels-alder reaction) – **Electrocyclic reactions-** Nazarov cyclisation – **Sigmatropic rearrangements** (Cope, Claisen, Oxy Cope- aza Cope and Sommelet-Hauser) and Cheletropic reactions.

UNIT-II ORGANIC PHOTOCHEMISTRY 18 Hours

2.1 Photo Chemistry- I

Interaction of electromagnetic radiation with matter-Excitation- the excited state- the transfer of excitation energy(sensitization and quenching)- **photoreduction**, **photoaddition :** photoaddition of alkene and alkynes to aromatic compounds-photoaddition of alkenene to carbonyl- Norrish Type-I & II. photodimerisation, Excimer, Exciplexes, Isomerisation of alkenes- Photostationery state, conjugated dienes and aromatic compounds **photo oxidation:** formation of peroxy compounds- oxidative coupling of aromatic compounds- Barton reaction

2.2 Photo Chemistry -II

Intramolecular reactions of carbonyl compound: Norrish type-I and Norrish type-II. – β-ϒ unsaturated carbonyl compounds. Intermolecular cyclo addition reactions-[2+2] cycloaddition reactions, Paterno – Buchi reaction- cycloaddition reactions of benzene. **Photo rearrangement:** cis-trans isomerisation-intramolecular photocyclisation-**sigmatropic rearrangements:** cyclohexadienone. **Photo chemical fragmentation:** Photolysis of diazoalkanes- alkyl azide-Barton reaction.

UNIT - III ADDITION REACTIONS 18 Hours

3.1 Addition to carbon-carbon multiple bonds-addition mechanism-electrophilic, nucleophilic and free-radical additions-cyclo addition, orientation and reactivity. Selected reactions - Birch reduction-catalytic semi reduction of alkynes - Hydroboration-selective hydroborating agents-oxymercuration-demercuration-epoxidation of alkene-Sharpless asymmetric epoxidation- Baeyer Villiger reaction- - Michael reaction.

3.2 Addition to carbon-hetero atom multiple bonds- addition orientation and reactivity -Selected name reactions - Acyloin ester condensation, Aldol condensation, Benzoin condensation, Cannizaro reaction, Claisen reaction, Darzen’s condensation, Knovenegal reaction, Mannich reaction and Stobbe condensation.

UNIT – IV CARBON-CARBON BOND FORMATION REACTIONS 18 Hours

4.1 Mechanistic details, stereochemical considerations and significance of the following reactions: Formation of carbon-carbon single bonds - Mitsunobu reaction- Reformatsky reaction - Robinson annulations - Stork Enamine alkylation- Gattermann and Gattermann-Kosch formylation reaction. **Formation of carbon-carbon double bonds** - Bamford-Stevens reaction- Horner-Wadsworth-Emmons reaction- Julia olefination-Perkin reaction. **Free radical reaction**-Hoffman-Loffler-Freytag reaction- Hundsdiecker reaction

4.2 Formation of carbon-carbon single bonds by organometallic reagents - Principles- Organo lithium compounds -LDA, R-Li- organomagnesium compounds – Organo copper compounds(Gilman’s reagent) – organo cadmium compounds – organomercury compounds- organozinc compounds. **Reagents containing sulfur, boron, silicon-** sulfur ylide,sulfoxonium ylide, 9-BBN, disiamyl borane, thexyl borane, trimethyl silyl iodide

UNIT-V REAGENTS FOR OXIDATION AND REDUCTION REACTIONS 18 Hours

5.1 Preparation, properties and characteristics of the following oxidizing agents and their reaction on alkenes, aromatic rings, ketones, ketals and carboxylic acids - Chromyl chloride, Periodic acid, Pyridinium Chloro Chromate -PCC, Dessmartin, Dichloro Dicyano hydro quinone -DDQ, iodobenzenediacetate, 2- iodoxybenzoic acid - IBX, sodium hypochlorite (bleach), Lead tetra acetate-$Pb(OAc)_4$

5.2 Preparation, properties and characteristics of the following reducing agents and their reactions on alkenes, alkynes, aromatic rings, carbonyls, Ketals, azo groups, epoxides and carboxylic acids - $LiAlH_4$, Lithium trialkylborohydride, DIBAL, tri-t butyloxyaluminium hydride, $NaBH_4$, sodium cyanoborohydride and hydrazine.

2B.Topics for Self-Study:

S. No	Topic	Weblink
1	Hetro diene-dienophile and Lewis acid mediated pericyclic reaction	https://nptel.ac.in/courses/104/106/104106077/
2	Photo induced electron transfer reaction	https://nptel.ac.in/courses/104/106/104106077/
3	Jacobsen-Katsuki-Epoxidation	http://www.namereactions.org/jacobsen-katsuki-epoxidation/
4	New Approaches to Alkene Functionalization via Dehydrogenative Metallation Catalyzed by First-Row Transition Metals	https://acswebcontent.acs.org/prfar/2014/Paper12948.html
5	Kornblum Oxidation Parikh-Doering Oxidation	http://www.iitg.ac.in/kbhabak/files/KPB_CH-420-Lectures%204_5-6_7.pdf

2C.Text Books:

1. Ratan Kumar Kar, “*Frontier Orbital and Symmetry Controlled Pericyclic Reactions*”, Books and Allied Ltd, 2009. (Unit-I)
2. Jagadamba Singh, “*Photochemistry and Pericyclic Reactions*” New Age; Third Edition 2012 (Unit I, II)
3. Jerry March, “ *Advanced Organic Chemistry – Reaction Mechanisms and Structure*”, Wiley India, 2006. (Unit-III, IV, V)
4. Richard O.C. Norman, James M. Coxon “*Principles of Organic Synthesis*” CRC Press (Special Indian Edition), 2017 (Unit-III, IV, V)

2D.Recommended Reference Books:

1. Jonathan Clayden, Nick Greeves, Stuart Warren, “*Organic Chemistry*” Oxford University Press, 2014.
2. James MorrissCoxon , Brian Halton “*Organic Photochemistry*”, Cambridge University Press, 2011.
3. W. Carruthers, “*Modern Methods of Organic Synthesis*”, Cambridge University Press,Cambridge , 2015.
4. Ahluwalia V K “*Organic Reaction Mechanism*” Narosa Publication, 2010.

5. S.M. Mukherji and S.P.Singh, “*Reaction Mechanism in Organic Chemistry*”, Macmillan India Ltd., Patna, 1990

3.Specific Learning Outcomes (SLO)

Unit	Course Contents	Learning Outcomes	Blooms Taxonomic levels of Transaction
I	**PERICYCLIC REACTIONS**		
1.1	Frontier Orbital Description	Construct FMO orbitals of organic molecules.	K3
	Correlation approach of – Woodward Hofmann rules Regiochemistry- Stereo chemical aspects- Endo/Exo selection - role of secondary orbital interaction in the following: **Diels Alder Reactions** (including 1,3 dipolar additions intramolecular reaction -the retro diels-alder reaction- asymmetric diels-alder reaction) **Electrocyclic reactions-** Nazarov cyclisation **Sigmatropic rearrangements** (Cope, Claisen, Oxy Cope- aza Cope and Sommelet-Hauser) and Cheletropic reactions.	Predict the stereo chemistry of the reaction products by making use of Woodward Hoffman rule and correlation diagram.	K3
		Plan and develop the mechanism for different types of pericyclic reaction.	K3
		Identify the theoretical feasibility of reactions at different conditions.	K3
II	**ORGANIC PHOTOCHEMISTRY**		
2.1	**Photo Chemistry- I**		
	Interaction of electromagnetic radiation with matter-Excitation- the excited state- the transfer of excitation energy(sensitization and quenching)	Describe the photochemical energy transfer of the reaction and its mechanism.	K2

	Photoreduction and **Photoaddition** Photoaddition of alkene and alkynes to aromatic compounds-photoaddition of alkenene to carbonyl- Norrish Type-I & II.	Classify photo chemical reactions and the product based on the structure of the substrate.	K4
	Photodimerisation Excimer, Exciplexes, Isomerisation of alkenes- Photostationery state, conjugated dienes and aromatic compounds	Describe Photodimerisation based on the structure of substrate and condition of the reaction.	K4
		Analyze the product ratios based on the energy transfer of photo isomerisation reaction	K4
	Photo oxidation: formation of peroxy compounds- oxidative coupling of aromatic compounds-Barton reaction	Explain the mechanism for various photo oxidation reactions.	K4
2.2	**Photo Chemistry –II**		
	Intramolecular reactions of carbonyl compound: Norrish type-I and Norrish type-II. – β-ϒ unsaturated carbonyl compounds. Intermolecular cyclo addition reactions-[2+2] cycloaddition reactions, Paterno – Buchi reaction- cycloaddition reactions of benzene.	Predict the type of photochemical reaction in carbonyl compounds.	K3
		Analyse the condition of reaction and structure of the substrate to solve problems related to Intra molecular reaction of Carbonyl compound.	K4
	Photo rearrangement: cis-trans isomerisation-intramolecular photocyclisation-**sigmatropic rearrangements:** cyclohexadienone.	Predict the structure of product based on the reaction condition and substrate structure.	K4
	Photo chemical fragmentation: Photolysis of diazoalkanes- alkyl azide-Barton reaction.	Identify the dissociation pattern in different N- based compounds.	K3
III	**ADDITION REACTIONS**		
	3.1 Addition to carbon-carbon multiple bonds		

	Addition mechanism-electrophilic, nucleophilic and free-radical additions-cyclo addition, orientation and reactivity	Distinguish types of addition reaction.	K4
		Predict the mechanism of addition reactions.	K3
		Illustrate the reaction product based on orientation and reactivity	K4
	3.2 Addition to carbon-hetero atom multiple bonds		
	Selected reactions - Birch reduction- catalytic semi reduction of alkynes - Hydroboration-selective hydroborating agents-oxymercuration-demercuration-epoxidation of alkene-Sharpless asymmetric epoxidation- Baeyer Villiger reaction- -Michael reaction.	Predict the mechanism for different reactions.	K5
		Evaluate different reactions based on the selectivity of reagent, nature of substrate structure and reaction condition.	K5
		Deduce the products of different reactions.	K5
IV	**CARBON-CARBON BOND FORMATION REACTION** **Mechanistic details, stereochemical considerations and significance of the following reactions:**		
	4.1 Formation of carbon-carbon single bonds		
	Mitsunobu reaction- Reformatsky reaction - Robinson annulations - Stork Enamine alkylation-Gattermann and Gattermann-Koschformylation reaction.	Predict the mechanism and the products of the reactions.	K5
		Evaluate the products obtained for the reactions based on the selectivity of reagent, nature of substrate structure and reaction condition.	K5
	Formation of carbon-carbon double bonds Bamford-Stevens reaction-Horner-Wadsworth-Emmons reaction- Julia olefination-Perkin reaction. Free radical mechanism	Predict the mechanism for different reactions.	K5
		Evaluate different reactions based on the selectivity of reagent, nature of substrate structure and reaction condition.	K5
		Plan a synthesis for the formation of C-C bond.	K4
	Hoffman-Loffler-Freytag reaction-Hundsdiecker reaction	Deduce the mechanism for different reactions.	K4

		Evaluate different reactions based on the selectivity of reagent, nature of substrate structure and reaction condition.	K5
		Plan a synthesis for the formation of C-C bond.	K4
4.2	**Formation of carbon-carbon single bonds by organometallic reagents** Principles- Organo lithium compounds -LDA, R-Li- organomagnesium compounds – Organo copper compounds(Gilman’s reagent) – organo cadmium compounds – organomercury compounds- organozinc compounds.	Write the mechanism for different reactions.	K5
		Evaluate different reactions based on the selectivity of reagent, nature of substrate structure and reaction condition.	K5
		Plan a synthesis for the formation of C-C bond.	K4
	Reagents containing sulfur, boron, silicon- sulfur ylide,sulfoxoniumylide, 9-BBN, disiamylborane, thexylborane, trimethylsilyl iodide	Write the mechanism for different reactions.	K5
		Design the synthesis for the formation of C-C bond using sulfur, boron and silicon based reagent.	K4
V	**REAGENTS FOR OXIDATION AND REDUCTION REACTIONS**		
5.1	**Preparation, properties and characteristics of the following oxidizing agents** : Chromyl chloride, Periodic acid, PyridiniumChloro Chromate - PCC, Dessmartin, DichloroDicyano hydro quinone - DDQ, iodobenzenediacetate, 2-iodoxybenzoic acid - IBX, sodium hypochlorite (bleach), Lead tetra acetate-$Pb(OAc)_4$	Predict the mechanism for different reactions.	K5
		Evaluate different reactions based on the selectivity of reagent, nature of substrate structure and reaction condition.	K5
		Compare the reactivity and selectivity of different oxidizing agents.	K5
		Choose the suitable reagent while planning synthesis.	K5
5.2	**Preparation, properties and characteristics of the following reducing agents and their**	Write the mechanism for different reactions.	K5

	reactions: LiAlH_4, Lithium trialkylborohydride, DIBAL, tri-t butyloxyaluminium hydride, NaBH_4, sodium cyanoborohydride and hydrazine.	Evaluate different reactions based on the selectivity of reagent, nature of substrate structure and reaction condition.	K5
		Compare the reactivity and selectivity of different reducing agents.	K5
		Choose the suitable reagent while planning synthesis.	K5
		Evaluate the reactivity of different boron based and metal based hydrides.	K5

4.Mapping Scheme for COs, POs and PSOs

L-Low M-Moderate H- High

Course Title: REACTIONS AND MECHANISMS IN ORGANIC CHEMISTRY
Course Code : P19CH205

Mapping	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PSO1	PSO2	PSO3	PSO4
CO1	H	H	H	M	L	-	L	-	M	H		H	L
CO2	H	H	H	M	H	L	-	-	H	H	H	M	L
CO3	H	H	H	M	H	M	M	-	H	-	H	M	
CO4	H	H	M	M	H	L	H	-	M	M	H	-	M
CO5	H	M	H	M	H	-	H	-	M	H	H	-	H
CO6	H	H	H	M	H	-	H	-	H	H	H	-	M

5.Course Assessment Methods

Direct

1. Continuous Assessment Test (Model Exams) I, II
2. Open book test; Cooperative learning report, Assignment; Journal paper review, Group Presentation, Project report, Poster preparation, Proto-type or Product Demonstration etc. (as applicable)
3. End Semester Practical Examination

Indirect

1. Course-end survey

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Elective Course - I

DATA ANALYSIS AND SELECTED ANALYTICAL TECHNIQUES

Semester: II **Code: P19CH2:1**
Credits: 4 **Total Hours: 75**
Hours/week:5

1.Course Outcomes:

After the successful completion of this course the students will be able to

S.No.	Course Outcomes	Level	Unit
1	Justify different hypothetical tests to confirm the reliability of measured data	K5	I
2	Explain the principle and applications of various electro analytical techniques	K4	II
3	Interpret the Chromatogram of different chromatographic techniques	K3	III
4	Analyze structure of molecules using analytical, spectral and microscopic techniques	K4	IV
5	Determine the Crystal parameters and the crystal structures	K5	V
6	Analyze the structural composition and morphology of molecules	K4	V

2A. Syllabus

UNIT -I **DATA ANALYSIS & IPR** **15 Hours**

1.1 Mean – Median – Standard deviation – Test of hypothesis T-test F-test - Correlation and Regression – Least Square method for curve fitting - Significant Figures in scientific measurements.

Handling numeric data: Spread Sheet software – Creating a Spread Sheet – Basic functions and formulae – Creating Charts, Tables and Graphs.

Xxxx- Revised content

1.2 Intellectual Property Rights (IPR): Introduction and the need for IPR – Patents – Copyrights – Trademarks – Geographical Indications – industrial Designs – IP Administration in India – Plagiarism and its Detection.

UNIT-II ELECTROANALYTICAL TECHNIQUES-I 15 Hours

2.1 Cyclic Voltammetry – Basic principle and Experimental technique, Types of Electrodes, Ion selective electrodes, Typical cyclic Voltammogram- reversible, irreversible and quasi-reversible systems.

2.2 Factors affecting limiting current – residual current, migration current, diffusion current (i_d), Kinetic current, half-wave potential, Ilkovic equation, - Applications example: electrochemical oxidation of ascorbic acid.

UNIT-III ELECTROANALYTICAL TECHNIQUES-II 15 Hours

3.1 Differential Pulse Voltammetry (DPV) – Basic principle and technique, applications. Analysis of metal ions in a mixture. Stripping Voltammetry.

3.2 Amperometry – Principle, Instrumentation, electrodes, titration curves and Applications.

UNIT–IV CHROMATOGRAPHIC TECHNIQUES 15 Hours

4.1. High Performance Liquid Chromatography (HPLC): Principle, Theory, Instrumentation. Various types – adsorption, partition (reverse phase), partition (normal phase), ion-exchange and size exclusion chromatography – detectors. Interpretation of detector output and Applications.

4.2 Gas Liquid Chromatography (GLC): Principle, Theory, Instrumentation – Description of the technique – Schematic diagram of a gas chromatograph, a typical chromatogram, detectors – flame ionization detector, electron capture detector and applications of GLC.

4.3 Gas Chromatography-Mass Spectrometry (GCMS): – Principle, theory, instrumentation and applications

UNIT – V Crystalline Structure and Surface Morphology 15 Hours

5.1 X-ray Diffraction Techniques - Crystal symmetry – Combination of symmetry elements – Crystal classes – Screw axis and Glide planes – diffraction pattern of crystalline and amorphous materials — Instrumentation of X-ray diffractometer – Examination of XRD pattern-Scherrer's equation – Calculation of Crystal size and prediction of planes – Determination of Cubic and Hexagonal Structures.

5.2 Scanning Electron Microscope (SEM) and Transmission Electron Microscope (TEM): Principle, Instrumentation and Applications.

5.3 Photo Electron Spectroscopy (PES), Electron Spectroscopy for Chemical Analysis (ESCA) and Auger Electron Spectroscopy: Principle, Techniques and applications.

2B.Topics for Self Study

Topics for Self StudyTopics	**Links**
AC polarography Cyclic Voltammetry	https://pubs.acs.org/doi/pdf/10.1021/acs.jchemed.7b00361 https://www.youtube.com/watch?v=utPPQZP_mrU
SEM	http://www.fhi-berlin.mpg.de/acnew/department/pages/teaching/pages/teaching_wintersemester_2009_2010/dangsheng_su_scanning_electron_microscopy_100129.pdf https://www.youtube.com/watch?v=GY9lfO-tVfE
TEM	https://www.youtube.com/watch?v=zkr3JmhjKbg
X-Ray Diffraction powder	https://www.youtube.com/watch?v=lwV5WCBh9a0
X-Ray Diffraction – single crystal	https://www.youtube.com/watch?v=suVNYD1nCm4
GC-Instrumentation	https://www.youtube.com/watch?v=PV4NYBUaUrQ
HPLC- Instrumentation	https://www.youtube.com/watch?v=kz_egMtdnL4
C Programming For Beginners	https://www.youtube.com/watch?v=8PopR3x-VMY

Xxxx- Revised content

2C.Text Books

1. H.H. Willard, L.L. Merritt and John A. Dean, “*Instrumental Methods of Analysis*”, CBS Publishers, 2004 **(Unit-I)**
2. R. Gopalan, P.S. Subramanian, K. Rengarajan, “*Elements of Analytical Chemistry*”, Sultan Chand and Sons, New Delhi, 1997. **(Unit II-IV)**
3. Doughlas A. Skoog, Donald M.West, F. Jeames Holler, Stanley, R.Crouch,“*Fundamentals of Analytical Chemistry*”, Thomas Books, Bangalore, 2004. **(Unit II - V)**

2D.Recommended Reference Books:

1. Gary D. Christian, “*Analytical Chemistry*”, John Wiley and Sons, Singapore, 2004.
2. B.K. Sharma, “*Instrumental Methods of Chemical Analysis*”, Goel Publishing House, Meerut,1999.
3. G.L.D. Krupadanam et al., “*Analytical Chemistry*”, University Press, Hyderabad, 2001.

3.Specific Learning Outcomes (SLO)

Unit	Course Content	Learning Outcomes	Blooms Taxonomic Levels of Transaction
	UNIT I: DATA ANALYSIS & IPR		
1.1	Mean – Median – Standard deviation – Test of hypothesis, T-test F-test	Analyse the data by different test of hypothesis	K4
	Correlation and Regression – Least Square method for curve fitting - Significant Figures in scientific measurements.	Compare different curve fitting methods	K4
		Examine the significant figures in scientific measurements.	K3

	Handling numeric data: Spread Sheet software – Creating a Spread Sheet – Basic functions and formulae – Creating Charts, Tables and Graphs.	Evaluate data by creating schematic charts	K5
1.2	Intellectual Property Rights (IPR): Introduction and the need for IPR	Describe about intellectual property rights	K2
	Patents – Copyrights – Trademarks	Compare the differences among patents, copyrights and trademarks	K2

Xxxx- Revised content

	Geographical Indications – industrial Designs – IP Administration in India	Illustrate the Geographical Indications, Industrial design and IP Administration in India	K2
	Plagiarism and its Detection.	Interpret the methods of plagiarism checking and detection.	K2
	UNIT II: ELECTROANALYTICAL TECHNIQUES-I		
2.1	Cyclic Voltammetry – Basic principle and Experimental technique, Types of Electrodes, Ion selective electrodes	Explain about experimental techniques of cyclic voltammetry	K2
		Classify the types of electrodes	K2
	Typical cyclic Voltammogram- reversible, irreversible and quasi-reversible systems.	Analyze cyclic voltammogram for reversible, irreversible and quasi-reversible processes	K4
2.2	Factors affecting limiting current – residual current, migration current, diffusion current (i_d), Kinetic current	Discuss the different factors, which are affecting limiting current	K2
	Ilkovic equation, - Applications example: electrochemical oxidation of ascorbic acid.	Inspect the Ilkovic equation to determine the concentration of electroactive species.	K4
		Deduce the mechanism of electrochemical reactions	K4
	UNIT III: ELECTROANALYTICAL TECHNIQUES-II		
3.1	Differential Pulse Voltammetry (DPV) – Basic principle and technique	Describe the principle and techniques of Differential Pulse Voltammetry.	K2
	DPV- Applications - Analysis of metal ions in a mixture	Analyze different metal ions from its mixture	K4
	Stripping Voltammetry	Relate the principle and quantitative determination of specific ions.	K2
3.2	Amperometry – Principle and Instrumentation techniques	Summarize the principle and instrumentation of Amperometry techniques	K2
	Applications of Amperometry	Experiment the electroactive species both qualitatively and quantitatively.	K4
	UNIT IV: CHROMATOGRAPHIC TECHNIQUES		
4.1	High Performance Liquid Chromatography (HPLC): Principle,	Discuss the principle and instrumentation of HPLC	K2

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	Theory, Instrumentation		
	Types – adsorption, partition (reverse phase), partition (normal phase), ion-exchange and size exclusion chromatography	Classify the different types of chromatographic techniques	K2
	Interpretation of detector output and Applications.	Interpret the chromatogram to separate, identify, and quantify each component in a mixture	K2
4.2	Gas Liquid Chromatography (GLC): Principle, Theory, Instrumentation– Description of the technique	Express the principle of GLC	K2
		Sketch the instrumentation of GLC	K3
	Schematic diagram of a gas chromatograph, a typical chromatogram	Review the different types of chromatograms	K2
	detectors – flame ionization detector, electron capture detector	Compare different detectors to evaluate different set of samples	K2
	Applications of GLC.	Construct the GLC technique chromatogram to separate, identify, and quantify vaporizable compounds	K3
	GCMS – Principle, theory, instrumentation, Applications	Report the principle, instrumentation and application of GCMS technique.	K3
	UNIT V: CRYSTALLINE STRUCTURE AND SURFACE MORPHOLOGY		
5.1	X-ray Diffraction Techniques : Crystal symmetry – Combination of symmetry elements - Crystal classes – Screw axis and Glide planes – diffraction pattern of crystalline and amorphous materials-	Relate symmetry elements with different forms of crystals.	K2
	Instrumentation of X-ray diffractometer	Discuss the instrumentation of X-ray diffractometer	K2
	Examination of XRD pattern- Scherrer's equation – Calculation of Crystal size and prediction of planes – Determination of Cubic and Hexagonal Structures.	Differentiate various types of crystal systems	K4

5.2	Scanning Electron Microscope (SEM) and Transmission Electron Microscope (TEM): Principle, Instrumentation and Applications	Explain the principle and instrumentation of SEM and TEM.	K3
		Correlate the SEM & TEM technique to explore the surface morphology and internal composition of materials	K4
5.3	Photo Electron Spectroscopy (PES), Electron Spectroscopy for Chemical Analysis (ESCA) and Auger Electron Spectroscopy: Principle, Techniques	Write the principle of PES, ESCA and Auger electron spectroscopy techniques.	K3

4.Mapping Scheme for the PO, PSOs and Cos

L-Low **M-Moderate** **H- High**

Course Title: DATA ANALYSIS AND SELECTED ANALYTICAL TECHNIQUES **Course Code: P19CH2:1**													
	PO 1	**PO 2**	**PO 3**	**PO 4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PSO1**	**PSO2**	**PSO3**	**PSO4**
CO1	H	H	M	-	H	H	L	H	H	H	-	H	-
CO2	H	-	-	H	-	-	H	-	-	M	L	-	H
CO3	H	H	H	H	M	-	M	-	H	-	H	M	H
CO4	H	H	M	H	H	-	H	-	-	H	-	H	H
CO5	H	H	-	H	-	H	L	M	H	M	-	H	H
CO6	H	H	H	H	-	L	L	M	H	-	-	H	H

5.Course Assessment Methods

DIRECT:

1. Continuous Assessment Test (Model Exams) I, II
2. Open book test; Cooperative learning report, Assignment; Journal paper review, Group Presentation, Project report, Poster preparation, Proto-type or Product Demonstration etc. (as applicable)
3. End Semester Practical Examination

INDIRECT:

1. Course-end survey

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Xxxx- Revised content

Core Practical - III

INORGANIC SEMIMICRO ANALYSIS & COLORIMETRIC ESTIMATIONS

Semester : II **Code : P19CH2P3**
Credits : 3 **Total Hrs : 90**
Hours /week:6

1.Course Outcomes :

At the end of this course, the students will be able to

S.No.	Course Outcomes	Level
1	Classify rare and common metal cations of different groups present in a mixture	K4
2	Develop analytical skills required for identifying and separating cations in a Mixture	K6
3	Choose appropriate reagents for the identification and separation of cations	K5
4	Analyze water and soil samples using the principles of Semimicro Qualitative Analysis	K4
5	Estimate metal ions colourimetrically	K5
6	Test the pollutant concentration in samples by constructing a standard graph applying Beer-Lambert's law	K6

2A. Syllabus

1. SEMI MICRO QUALITATIVE ANALYSIS

Analysis of a mixture containing two common and two rare cations:
Common Cations: I group - Pb, Tl, II group – Cu, Cd, Bi **,** III group – Al, Fe, IV group – Mn, Zn, Co, Ni, V group – Ca, Sr, Ba, VI group – Mg, Zero group - NH_4^+ ..
Rare Cations - I group – W, Ti, IA group – Se, Te, II group – Mo,
III group – Be, Zr, Ce, V, U, VI group - Li .

2. COLOURIMETRIC ESTIMATION

Estimation of Copper, Ferric ion, Nickel, Chromium and Manganese using Photoelectric colourimeter

Xxxx- Revised content

2B.Text Book :

1. V. Ramanujam, “Inorganic Semimicro Qualitative analysis”, 3rd Edition, The National Publishing Company, Chennai 1974.

2C.Reference Books:

1. Vogel’s, “Text book of Inorganic Qualitative Analysis”, 4th Edition. ELBS, 1974.

3.Specific Learning Outcomes (SLO)

S.No	**Course Content**		**Learning Outcomes**	**Blooms Taxonomic levels of Transaction**
1	**Semimicro Qualitative Analysis**		Analyze common and rare cations systematically in a given inorganic mixture by semi-micro qualitative analysis.	K4
	I	Pb, W		
	I A	Se, Te	Categorize the given ions into their respective groups.	K4
	II A	Cu, Cd, Bi	Develop analytical skills required for identifying cations in a mixture.	K6
	II B	Mo		
	III	Be, Zr, Ce, V,U	Distinguish inter and intra group precipitation and separation techniques.	K4
	IV	Zn, Mn, Ni, Co		
	V	Ca, Ba, Sr		
	VI	Mg, Li		
2	**Colourimetric Estimations** Estimation of Copper, Estimation of Ferric ion, Estimation of		Apply the principle of colourimetry in the quantitative estimation of metal ions.	K3
			Construct a standard graph	K3

	Nickel, Estimation of Chromium Estimation of Manganese	Estimate colourimetrically the metal ions.	K5
		Test the pollutants concentration in contaminated samples by constructing a standard graph applying Beer-Lambert’s law	K6
		Correlate concentration of the solution and absorbance of the solution.	K4

4.Mapping Scheme for the PO, PSOs and Cos

L-Low M-Moderate H- High

Course Title: INORGANIC SEMIMICRO ANALYSIS & COLORIMETRIC ESTIMATIONS
Course Code : P19CH2P3

Mapping	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PSO1	PSO2	PSO3	PSO4
CO1	M	H	L	M	M	-	M	M	-	H	H	M	L
CO2	M	L	L	M	M	-	M	M	-	H	H	L	H
CO3	H	M	M	M	M	-	M	L	-	HM	H	M	H
CO4	M	H	H	H	M	M	L	H	L	M	H	M	H
CO5	M	H	L	H	M	-	M	M	-	H	M	M	H
CO6	L	H	M	M	H	H	-	M	-	M	-	M	H

5.COURSE ASSESSMENT METHODS

Direct

1. Continuous Internal Assessment
2. Model Exam 1 & 2
3. Viva -Voce
4. End Semester Examination

Indirect

1. Course-end survey

Core Practical - IV QUANTITATIVE ANALYSIS OF ORGANIC COMPOUNDS

Semester: III **Code: P19CH2P4**
Credits: 3 **Total Hrs: 90**
Hours /week:6

1.Course outcome:

At the end of this course, the student will be able to:

S.No.	Course Outcomes	Level
1	Estimate organic compounds volumetrically	K5
2	Separate the components in organic mixture by paper chromatographic technique	K4
3	Choose the suitable method for purification of organic compounds	K5
4	Recommend appropriate solvents for recrystallization technique	K5
5	Estimate the amount of protein present in milk	K4
6	Compare the saponification value of different oils	K5

2A. Syllabus

1. QUANTITATIVE ANALYSIS

1. Estimation of Phenol / Aniline.
2. Estimation of Amide.
3. Estimation of Glucose. (Methylene Blue Method)
4. Estimation of Ethyl methyl ketone.
5. Estimation of Saponification value of oil.
6. Estimation of Nitro group.
7. Estimate the given quantity of glycine
8. Estimation of Ester group.

2. PAPER CHROMATOGRAPHIC TECHNIQUES

1. Identification of Amino acids by Paper Chromatogaphy.
2. Separation of the mixture of three dyes by two dimensional Paper Chromatography.
3. Separation of the mixture of three dyes by radial Paper Chromatography.

3. ISOLATION

1. Isolation of Casein from the given quantity of Milk

4. DISTILLATION & RECRYSTALLISATION

1. Distillation of the mixture of organic liquids and determination of Boiling points.
2. Recrystallisation of organic solid and determination of Melting points of the crude and the Pure Compound.

2B.Reference Books:

1. Syed Mumtazuddin, Organic Chemistry – A Laboratory Manual, Narosa Publishing House,New Delhi,2014.
2. Syed Mumtazuddin,Advanced Practical Chemistry, Syed Mumtazuddin,Pragati Prakashan, Meerut, 2014
3. V K Ahluwalia & Sunita Dhingra, Advanced Experimental Organic Chemistry, Manakin Press, New Delhi, 2017.

3.Specific Learning Outcomes

.No	Course content	Learning Outcomes	Blooms Taxanomic Levels of Transactions
	Quantitative Analysis		
1	Estimation of Phenol / Aniline.	Estimate phenol and aniline bybromination method.	K5
2	Estimation of Amide	Test the amide content and to evaluateits concentration	K5
3	Estimation of Glucose. (Methylene Blue Method)	Estimate glucose by methylene bluemethod.	K5
4	Estimation of Ethyl methyl ketone	Estimate ketone by haloform method.	K5
5	Estimation of Saponification value of oil.	Compare the saponification values ofdifferent oils.	K5
6	Estimation of Nitro group	Determine the nitro group of the givensample by reduction method.	K5
7	Estimate the given quantity of glycine	Estimate glycine by colorimetry method.	K5
8	Estimation of Ester group	Estimate ester by hydrolysis method.	K5
	Paper Chromatographic Techniques		

9	Identification of Amino acids by Paper Chromatography.	Develop a method to separate mixture ofamino acid and dyes by paper chromatographic method.	K4
10	Separation of the mixture of three dyes by two dimensional Paper Chromatography.		
11	Separation of the mixture of three dyes by radial Paper Chromatography		
	Isolation		
12	Isolation of Casein from the given quantity of Milk	Isolate casein from milk samples.	K3

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	Distillation & Recrystallisation		
13	Distillation of the mixture of organic liquids and determination of Boiling points.	Separate organic liquid mixture by distillation method and to check purity of the sample by determination of its boiling point.	K3
14	Recrystallisation of organic solid and determination of Melting points of the crude and the Pure Compound	Test the melting point of crude and pure compound to examine the suitable recrystallization methods.	K5
		Choose the correct solvent system for crystallization of organic solid.	K5
		Check purity of organic compound by determination of its melting point.	K5

4.Mapping Scheme for the PO, PSOs and Cos

L-Low **M-Moderate** **H- High**

Course Title : QUANTITATIVE ANALYSIS OF ORGANIC COMPOUNDS
Course Code: P19CH2P4

Mapping	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PSO1**	**PSO2**	**PSO3**	**PSO4**
CO1	H	H	H	**M**	**H**	-	M	**-**	**H**	**H**	**M**	**-**	**H**
CO2	H	H	H	**H**	**H**	-	H	**-**	**H**	**H**	**H**	**M**	**H**
CO3	H	H	H	H	H	-	H	M	H	H	H	-	H
CO4	H	H	H	H	H	-	H	M	H	H	H	-	H
CO5	H	H	H	H	H	-	H	M	H	H	H	M	H
CO6	H	H	H	H	H	-	H	M	H	H	H	M	H

5.COURSE ASSESSMENT METHODS

Direct

1. Continuous Internal Assessment
2. Model Exam 1 & 2
3. Viva -Voce
4. End Semester Examination

Indirect

1. Course-end survey

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PRACTICAL PREPARATORY COURSE -II

(For Organic and Inorganic Practical)

SEMESTER: II **TOTAL HOURS: 15**

Course Code: P19CH2P3 and P19CH2P4

COURSE OBJECTIVES:

- To understand the principles behind the experiments in **P19CH2P3 and P19CH2P4**
- To identify methods by which error may be reduced in experiments

UNIT - I ERRORS IN ANALYSIS AND MEASUREMENTS

Chemical analysis- sampling - types of analysis- limitations of analytical methods- accuracy-precision -types of errors- minimization of errors- significant figures- Principles of Organic estimations- Back titrations –Reactions involved in each step of estimation.

UNIT - II GOOD LABORATORY PRACTICES

Calibration and use of glass wares- Storing and recycling of some reagents in laboratory - Protocols for Handling chemicals and their disposal - Safety measures and first aid in the laboratory- Handling hazards due to strong acids and bases, toxic chemicals, Remedies for Ingestion, Inhalation and direct absorption of chemicals.

UNIT- III PRINCIPLES OF COLORIMETRIC ANALYSIS

A brief recollection of the Laws of Colorimetry – Components and Instruments of a Colorimeter – Mathematical expression and Importance of Absorbance, molar absorptivity – percentage transmittance – Construction of standard graph – extrapolation and interpolation. Preparation of some important organic and inorganic complexing agents.

UNIT - IV PRINCIPLES OF QUALITATIVE ANALYSIS

Rare and common ions – Grouping of ions – principles behind separation of ions into groups – common ion effect – Solubility Product – Group reagents and reactions involved.

TEXT BOOK:

1. V. Ramanujam, “Inorganic Semimicro Qualitative analysis”, 3rd Edition, The National Publishing Company, Chennai, 1974.

REFERENCES:

1. A.K. Srivastva, “Instrumental Approach to Chemical Analysis”, 4th Edition, S. Chand and Company, New Delhi, 2010.

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Core Course: VI **ORGANIC SPECTROSCOPY**

Semester: III **Code: P19CH306**
Credits: 5 **Total Hrs: 90**
Hours/week:6

1.Course Outcomes

After the successful completion of this course the students will be able to

S.No.	Course Outcomes	Level	Unit
1	Analyze the ultraviolet spectra of organic compounds	K4	I
2	Predict the absolute configuration of organic compounds through ORD & CD techniques	K5	II
3	Analyze IR Spectra of various organic compounds pertaining to functional groups and nature of bonding	K4	III
4	Interpret NMR (^{1}H, ^{13}C & 2D) spectra for structural elucidation of organic molecules	K5	IV
5	Decide the structure of organic molecules based on fragmentation pattern derived from mass spectra	K5	V
6	Justify the structure of the organic compounds using UV, IR, NMR and Mass spectral data	K5	V

2A. Syllabus

UNIT – I **Ultraviolet spectroscopy, ORD and CD** **18hours**

1.1 Ultraviolet spectroscopy - Various electronic transitions (185 - 800 nm), Beer –Lambert Law, effect of solvent on electronic transitions, UV bands for carbonyl compounds, unsaturated carbonyl compounds, dienes , conjugated polyenes. Fischer – Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Streic effect in biphenyls.

1.2 Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD) - Definition, deduction of absolute configuration, octant rule for ketones, Cotton effect and ORD curves. Comparison between ORD and CD and their interrelationships.

UNIT– II **FT-IR spectroscopy** **18hours**

FT-IR spectroscopy - Instrumentation and sample handling. Characteristic vibrationalfrequencies of alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of

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hydrogen bonding and solvent effect on vibrational frequencies , over tones, combination bands and Fermi resonance,

UNIT–III Nuclear Magnetic Resonance Spectroscopy 18hours

NMR- General introduction and definition, chemical shift, spin – spin interaction, shielding mechanism. Chemical shift values and chemicalexchange, effect of deuteration, complex spin-spin interaction between two, three, four, and five nuclei (first order spectra), virtual coupling, coupling constant. Simplification of complexspectra using - nuclear magnetic double resonance, contact shift reagents - solvent effects.Fourier transform technique - Nuclear Overhauser effect (NOE).

UNIT–IV ^{13}C-NMR Spectroscopy and 2D-NMR Spectroscopy 18hours

4.1 ^{13}C-NMR Spectroscopy - General considerations, chemical shift - Empirical calculation of chemical shift of aliphatic, Olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon .

2D NMR spectroscopy – principles and applications of COSY, NOESY, DEPT, INEPT, APT, and INADEQUATE techniques.

UNIT–V Mass Spectrometry 18hours

5.1 Mass Spectrometry **-** Introduction, ion production – Electron Ionisation (EI), Chemical Ionisation (CI), Field Desorption (FD) and Fast Atom Bombardment (FAB), factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

5.2 A review of spectroscopic problems - Calculation of double bond equivalent and its application in structure elucidation. Structural elucidation of organic molecules involving IR, UV, NMR and mass data.

2B.Topics for Self-Study:

S.No.	Topics	Web Links
1	Characterisation Techniques of polymers, nanocomposites and biomaterials	https://www.sciencedirect.com/topics/chemistry/uv-vis-spectroscopy
2	Two-Dimensional Infrared (2D IR) Spectroscopy: Theory and Applications-	https://doi.org/10.1366%2F0003702904087398
3	Advanced NMR techniques for structural characterization of heterocyclic structures	https://www.researchgate.net/publication/228591578
4	^{13}C NMR spectroscopy applications to brain energy metabolism	https://www.frontiersin.org/articles/10.3389/fnene.2013.00009/full
5	Advanced mass spectrometry-based methods for the analysis of conformational integrity of biopharmaceutical products	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3375681/

2C.Text Books

1. P.S. Kalsi, "Spectroscopy of Organic Compounds" , New Age International , New Delhi, 2016 **(Unit I-V)**
2. Y.R. Sharma, " Elementary Organic spectroscopy- Principles and chemical Applications", S.Chand & Co., New Delhi,2013. **(Unit I-V)**

2D.Reference Books

1. R.M. Silverstein, G.C. Bassier and T.C. Morrill, " Spectrometric Identification of Organic Compounds" , Wiley, New Delhi, 2015.
2. Donald L. Pavia, Gary M. Lampman, George S. Kriz "Introduction to Spectroscopy" Cengage Learning India Private Limited, 2015.
3. J.R. Dyer, "Application of Spectroscopy of Organic Compounds", Prentice Hall, New Delhi, 1978.
4. W.Kemp , " Organic spectroscopy " , Palgrave , New York, 2008.

3. **Specific Learning Outcomes (SLO)**

Unit	**Course Content**	**Learning Outcomes**	**Blooms Taxonomic levels of Transaction**
	Unit-1: Ultraviolet Spectroscopy, Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)		
1.1	**Ultraviolet Spectroscopy:** Various electronic transitions (185 - 800 nm)	Classify the various electronic transitions and compare their energies	K2
	Beer – Lambert Law	Categorize high and low intensity absorptions	K4
		Analyse the molar absorptivityand absorbance of the organic compound from given data	K4
	Effect of solvent on electronic transitions	Explain the dependence of solvent polarity on the wave length of absorption	K2
	UV bands for carbonyl, unsaturated carbonyl, dienes, conjugated polyenes compounds. Fischer – Woodward rules for conjugated dienes and carbonyl compounds	Evaluate the wavelengths of absorption of the organic compound through the set of empirical rules/values	K4
	Ultraviolet spectra of aromatic and heterocyclic compounds	Illustrate the characteristic electronic transitions of aromatic and heterocyclic compounds	K2
	Steric effect in biphenyls	Interpret the structural dependency on the absorption of energy for substituted biphenyls	K2
1.2	**Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)**	Relate the utility of ORD to deduct absolute configuration of	K2

	Definition of Optical Rotatory Dispersion (ORD)	organic compounds	
	Cotton effects and ORD curves. Octant rule for ketone - Deduction of absolute configuration	Predict the absolute configuration of organic compound from the given information.	K5
	Circular Dichroism	Explain the phenomenon andrelate its utility to the deduction of absolute configuration of organic compounds	K4
	Comparison between ORD and CD and their interrelationships	Compare the features of the respective techniques and explain their inter-relationship	K2
	Unit-2: FT-IR spectroscopy		
2.1	Instrumentation and sample handling	Recall the theory of electromagnetic spectrum and the criterion for organic compounds to absorb in infra-red region	K1
	Characteristic vibrational frequencies of organic functional groups (alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines)	Categorize various absorption frequencies with respect to the functional group and vice versa	K4
	Vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds)	Categorize various absorption frequencies with respect to carbonyl functional group and vice versa	K4
2.2	Effect of hydrogen bonding and solvent effect on vibrational frequencies	Apply the dependency and effect of H-bonding in the frequencies of absorption	K3
	Overtones, combination bands and Fermi resonance	Identify various bands in IR spectra of organic compounds	K2
	Unit-3: Nuclear Magnetic Resonance Spectroscopy		

3.1	Introduction and definition, chemical shift, spin- spin interaction	Identify the nuclear spin states, magnetic moments and mechanism of absorption of energy by the nucleus	K2
	Shielding mechanism - Chemical shift values	Differentiate the nature of shielding in the organic compound	K4
		Distinguish protons of various chemical shifts arising from different chemical environments	K5
		Assess the correlation for proton chemical shifts	K5
	Chemical exchange	Explain the nature of chemically exchangeable protons	K2
	Effect of deuteration	Illustrate deuterium isotopic effect	K2
	Complex spin-spin interaction between two to five nuclei (first order spectra) - Coupling Constant and Virtual Coupling	Identify magnetically equivalent and non-equivalent protons	K2
		Evaluate the splitting pattern dueto through-bond interactions when different kinds of magneticallynon-equivalent nuclei are present	K5
		Infer the stereochemical dependency of spin interactions in organic compounds	K4
	Simplification of complex spectra using – double resonance, contact shift reagents - solvent effects. Fourier Transform Technique - Nuclear Overhauser effect	Predict complex NMR spectra by applying various techniques	K5
	Unit-4: ^{13}C-NMR and 2D-NMR Spectroscopy		
4.1	Chemical shift - Empirical calculation of chemical shift of aliphatic, Olefinic, alkyne, aromatic, hetero-	Describe the theory of C-13 NMR spectra	K1

	aromatic and carbonyl carbon	Infer the chemical shifts of various organic functional groups using available empirical data	K4
		Predict the structure of the organic compound from the given C-13 NMR data/spectra	K5
4.2	2D NMR spectroscopy – principles and applications of COSY, NOESY, DEPT, INEPT, APT, and INADEQUATE techniques	Predict the structure of complex organic molecules by comparing through space coupling interactions	K5
	Unit-5: Mass Spectroscopy & Review of spectroscopic problems		
5.1	**Mass Spectroscopy** Electron Ionisation (EI), Chemical Ionisation (CI), Field Desorption (FD) and Fast Atom Bombardment (FAB) techniques	Compare the various modes of ionization techniques in mass spectroscopy	K2
	Factors affecting fragmentation, ion analysis, ion abundance	Identify the various factors affecting fragmentation of organic compounds in mass spectroscopy	K2
	Mass spectral fragmentation of organic compounds with common functional groups, molecular ion peak, metastable peak	Illustrate the various fragmentation patterns arising from the common functional groups	K4
	McLafferty rearrangement	Analyse the characteristic fragmentation to arrive atstructural aspects of organic compounds	K4
	Nitrogen rule	Predict the presence or absence of nitrogen based on the molecularion peak	K3
	High resolution mass spectrometry	Express the principles of the	K2

		techniques involved	
	Mass spectral fragmentation of organic compounds with respect to their structure determination	Predict the structure of organic compound by mass spectral fragmentation patterns	K5
5.2	**Review of spectroscopic problems:** Calculation of double bond equivalent and its application in structure elucidation. Structural elucidation of organic molecules involving IR, UV, NMR and mass data	Evaluate the spectral patterns of various organic compounds	K5

4.Mapping (CO, PO, PSO)

L-Low **M-Moderate** **H- High**

Course Title: ORGANIC SPECTROSCOPY
Course Code:P19CH306

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PSO1**	**PSO2**	**PSO3**	**PSO4**
CO1	H	H	H	H	H	-	H	M	L	H	L	L	L
CO2	H	H	M	L	L	-	L	L	L	H	M	M	M
CO3	H	H	H	H	H	-	H	M	M	H	H	H	H
CO4	H	H	M	H	H	-	M	M	M	H	H	H	H
CO5	H	H	M	H	M	-	M	M	M	H	H	H	H
CO6	H	H	M	H	M	-	H	M	H	H	H	H	H

5.Course Assessment Methods

DIRECT:

1. Continuous Assessment Test (Model Exams) I, II
2. Open book test; Cooperative learning report, Assignment; Journal paper review, Group Presentation, Project report, Poster preparation, Proto-type or Product Demonstration etc. (as applicable)
3. End Semester Practical Examination.

INDIRECT:

1. Course-end survey

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Core Course -VII THERMODYNAMICS AND ELECTROCHEMISTRY

Semester: III **Code: P19CH307**
Credits: 5 **Total Hrs: 90**
Hours/week:6

1.Course Outcomes:

After the successful completion of this course, the students will be able to

S.No.	Course Outcomes	Level	Unit
1	Evaluate the macroscopic properties using classical thermodynamics	K5	I
2	Analyze the fundamental concepts of atoms and molecules and their arrangements in different energy levels by statistical approach	K4	II
3	Determine the macroscopic properties based on the translational, vibrational, rotational and electronic partition functions of molecules	K5	III
4	Explain the electrochemical phenomena of various energy storage systems	K4	IV
5	Predict the mean ionic coefficient of different electrolytes and working principle of electrochemical cells and electrodes	K5	IV
6	Justify the electro kinetic phenomena of processes at electrodes	K5	V

2A. Syllabus

UNIT –I CLASSICAL THERMODYNAMICS 18 Hours

1.1 Partial molar properties–chemical potential, relationship between partial molar quantities and thermodynamic functions - Gibbs-Duhem equation-calculation of partial molar quantities from experimental data,

1.2 Thermodynamic properties of real gases-activity- fugacity concept - calculation of fugacity of real gas and activity coefficient –definition and experimental determination of activity coefficients of non-electrolytes.

UNIT –II STATISTICAL THERMODYNAMICS – I 18 Hours

2.1 Probability – types of events-theories of probability- multiplicative nature of probability-permutations and combinations – Stirling's Approximation.

2.2 Statistical mechanics – calculation of thermodynamic probability of system – Assembly , ensembles, phase space-definition of micro and macro states - different methods of counting macro and micro states – distinguishable and indistinguishable particles-classical statistics - derivation of Maxwell Boltzmann distribution law- Its application to gaseous system – energy, velocity distribution - concept of negative Kelvin temperature.

2.3 Quantum statistics-Bose Einstein and Fermi Dirac statistics-comparison with Maxwell-

Boltzmann statistics – application of BE statistics to photon gas-Application of FD statistics to electron gas and to thermionic emission – derivation of thermionic energy.

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UNIT- III STATISTICAL THERMODYNAMICS – II 18 Hours

3.1 Partition function – characteristics - translational, rotational, vibrational, electronic partition function - expression for enthalpy, internal energy, Gibb's energy, entropy (Sackur – Tetrode equation), work function and equilibrium constant in terms of partition functions – partition function of mono atomic and diatomic molecules.

3.2 Heat capacity of solids –Derivation of Einstein's equation and its limitations, Debye T - cubed law and its significance.

3.3 Non-equilibrium thermodynamics, Steady-State-phenomenological laws and Onsager's reciprocal relations.

UNIT-IV ELECTROCHEMISTRY-I 18 Hours

4.1 Debye-Huckel-Onsager theory and its derivation –Debye –Falkanhagen and Wein's effects – extension to Debye-Huckel Onsager theory.

4.2 Activity of ions in solutions-mean ionic activity coefficients-experimental determination – Debye-Huckel limiting law-modification for higher concentrations – Bjerrum model.

4.3 Electrochemical cells-Electrode –Electrolyte equilibrium-thermodynamic quantities from emf data – Nernst equation for electrode potential and emf of a cell – classification of electrodes(electrodes of I kind, II kind, redox and membrane) – electrolyte concentration cells (with and without transference) – liquid junction potential – its elimination – applications of concentration cells.

4.4 Electrochemical energy storage systems- primary and secondary cells-Fuel cells (efficiency- advantage-types)

UNIT-V ELECTROCHEMISTRY – II 18 Hours

5.1 Electrical double layer – theory of multiple layers at electrode- (Guoy Chapman, Stern and Helmholtz model) – double layer capacity – Electrokinetic phenomena, zeta potential and electro osmotic velocity, zeta potential and streaming potential – determination of zeta potential and interpretation of zeta potential values.

5.2 Process at electrodes-Butler-Volmer equation-high and low field approximation-Tafel equation

5.3 Electrochemical corrosion of metals, constructions and use of Pourbaix and Evans Diagrams and prevention of corrosion.

2B.Topics for Self-Study

S.NO	Topics	Web links
1	Fugacity of a gas in a Gaseous mixture and liquid in a liquid mixture	http://pillars.che.pitt.edu/files/course_17/print/Fugacity_and_Equilibrium_Calculations.pdf https://www.youtube.com/watch?v=t2UmK5tyWoU&ab_channel=Ch-11ChemicalEngg%2CChemistryandothers
2	Applications of Quantum Statistics	http://quantum.lassp.cornell.edu/lecture/quantum_statistical_mechanics
3	Partition function of real gas	http://www.tkm.kit.edu/downloads/ss2014_theof/Theory_F_2014.pdf
4	Types of Fuel cell	https://www.energy.gov/eere/fuelcells/types-fuel-cells
5	Different Types of Corrosion - their Causes and their Prevention	https://www.brighthubengineering.com/manufacturing-technology/81750-corrosion-prevention-techniques/ https://www.youtube.com/watch?v=A_rI9rNVgR8&ab_channel=MagicMarks

2C.Text Books:

1. M.C.Gupta, "Statistical Thermodynamics", Wiley Eastern Ltd., New Age International, New Delhi, 1998. **(Unit -II, III)**
2. R.P. Rastogi and R.R. Mishra, "An introduction to Chemical Thermodynamics", Vikas Publishing House, New Delhi, 2000. **(Unit -I, II, III)**
3. B.R. Puri, L.R.Sharma and M.S. Pathania, "Principles of Physical Chemistry", Vishal Publishing Co., Jalandar, 2017. **(Unit –IV, V)**

2D.Recommended Reference Books:

1. R. Stephen Berry, Stuart A.Rice and John Ross, "Physical Chemistry", Oxford University Press, New York, 2000.
2. D.A. Mcquarrie, J.D. Simon, "Molecular Thermodynamics", University Science books, California, 1999.
3. F.W.Sears, Thermodynamics, "Kinetic theory of Gases and statistical mechanics", 2nd Edition, Wesley, 1972.
4. Horia Metiu, "Physical chemistry- Thermodynamics", Taylor and Francis, 2006.
5. Peter Atkins and Julio de Paula Atkins "Physical Chemistry", Oxford University Press, Oxfored, 2018.
6. G.W.Castellan, "Physical Chemistry", Narosa Publishing House, New Delhi, 2002.
7. Robert J. Silbey, Robert A. Alberty, "Physical Chemistry", John Wiley and Sons,New York, 2006.

8. Philip Mathews, “Advanced Chemistry”, Foundation Books, New Delhi, 2003.
9. P.K. Ghosh, “Introduction to Photoelectron spectroscopy”, John Wiley and Sons, New York , 1989.

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10. Samuel Glasstone, “Introduction to Electrochemistry”, Prentice Hall, New Delhi, 2006.
11. D.R. Crow, “Principles and Applications of Electrochemistry”, Chapman and Hall, London, 1994.

3.Specific Learning Outcomes (SLO)

Unit	**Course Content**	**Learning outcomes**	**Blooms Taxonomic levels of Transaction**
	Unit –I Classical Thermodynamics		
I	Partial molar properties–chemical potential, relationship between partial molar quantities and thermodynamic functions	Solve the problems based on chemical potential determination	K3
	Gibbs-Duhem equation- calculation of partial molar quantities from experimental data	Deduce Gibbs-Duhem equation	K4
		Calculate partial molar properties	K4
	Thermodynamic properties of real gases- activity- fugacity concept - calculation of fugacity of real gas	Solve the problems based on fugacity	K4
	Activity coefficient –definition and experimental determination of activity coefficients of non-electrolytes.	Evaluate the activity coefficient of non- electrolytes	K5
	Unit-II Statistical Thermodynamic-I		
2.1	Probability – types of events-theories of probability- multiplicative nature of probability	Illustrate the types of events in probability	K2
		Summarize the theories of probability	K2
	Permutations and Combinations	Solve the permutation and combination problems	K3
	Stirling’s Approximation	Apply Stirling’s approximation to large systems	K3

2.2	Statistical mechanics – calculation of thermodynamic probability of system	Examine thermodynamic probability of system	K4
		Evaluate the most probable distribution	K4
	Assembly , ensembles, phase space-definition of micro and macro states	Compare the types of ensembles	K2
	Different methods of counting macro and micro states	Solve problems based on microstate and microstate counting	K3
		Evaluate statistical weight factor	K3
	Distinguishable and indistinguishable particles	Differentiate distinguishable and indistinguishable particles	K2
	Classical statistics - derivation of Maxwell Boltzmann distribution law- Its application to gaseous system – energy, velocity distribution - concept of negative Kelvin temperature.	Infer the significance of Maxwell Boltzmann distribution law	K3
		Apply Boltzmann distribution law in the calculation of properties of system	K3
2.3	Quantum statistics-Bose Einstein and Fermi Dirac statistics-comparison with Maxwell- Boltzmann statistics – application of BE statistics to photongas- Application of FD statistics to electron gas and to thermionic emission – derivation of thermionic energy.	Deduce Bose-Einstein and Fermi Dirac statistics	K4
		Compare three statistical thermodynamics	K2
		Explain Bose- Einstein condensation	K2
		Evaluate the energy involved in thermionic emission	K4
	Unit-III Statistical Thermodynamics-II		

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3.1	Partition function – characteristics - translational, rotational, vibrational, electronic partition function	Manipulate the values of partition functions and to arrive the numerical values	K3
		Calculate all types of partition functions for diatomic molecules	K3
		Compute thermodynamic parameters of system based on partition functions	K3
	Expression for enthalpy, internalenergy, Gibb's energy, entropy (Sackur – Tetrode equation), workfunction and equilibrium constant in terms of partition functions .	Relate thermodynamic functions with statistical thermodynamic function like partition functions	K3
		Deduce the Sackur-Tetrode equation	K4
		Compute Statistical entropy	K3
	Partition function of mono atomic and diatomic molecules	Evaluate the partition function of mono and diatomic molecules	K5
3.2	Heat capacity of solids –Derivation of Einstein's equation and its limitations, Debye T - cubed law and its significance.	Infer Einstein equation and Debye Equation	K4
		Calculate heat capacity of solids	K3
3.3	Non-equilibrium thermodynamics, Steady-State-phenomenological laws and Onsager's reciprocal relations.	Explain Onsager's reciprocal relation	K4
	Unit-IV Electrochemistry-I		

4.1	Debye-Huckel-Onsager theory and its derivation –Debye –Falkanhagen and Wein’s effects – extension to Debye-Huckel Onsager theory.	Interpret Debye-Huckel-Onsager theory	K3
		Explain Debye-Falkanhagen and Wein’s effect	K4
4.2	Activity of ions in solutions-mean ionic activity coefficients-experimental determination	Manipulate mean ionic activity coefficients of solutions	K3
	Debye-Huckel limiting law-modification for higher concentrations – Bjerrum model.	Deduce Debye-Huckel limiting law	K4
		Illustrate the primary and secondary salt effect	K4
		Analyze the influence of ionic strength	K4
4.3	Electrochemical cells-Electrode – Electrolyte equilibrium-thermodynamic quantities from emf data	Calculate EMF of a cell	K3
		Construct a cell diagram	K3
	Nernst equation for electrode potential and emf of a cell	Deduce Nernst Equation	K4
		Write a EMF Series	K3
		Evaluate the feasibility of cell reaction	K5
	Classification of electrodes(electrodes of I kind, II kind, redox and membrane)	Classify the types of electrodes with examples	K2
	Electrolyte concentration cells (with and without transference) – liquid junction potential – its elimination – applications of concentration cells.	Compare concentration cell with and without transference relation	K4
		Assess liquid junction potential	K5
		Compute Liquid junction potential of concentration cells	K3
		Write the applications of concentration cells	K3
4.4	Electrochemical energy storagesystems-primary and secondary cells- Fuel cells(efficiency-advantage-types)	Differentiate the types of energy storage system	K4
		Categorize energy storage cells	K4
	Unit-V Electrochemistry-II		

Xxxx- Revised content

5.1	Electrical double layer – theory of multiple layers at electrode- (Guoy Chapman, Stern and Helmholtz model) – double layer capacity	Compare the significance of double layer theory with multiple layer theory	K5
	Electrokinetic phenomena, zetapotential and electro osmotic velocity, zeta potential and streaming potential	Examine the relation between electro kinetic phenomena	K3
	Determination of zeta potential and interpretation of zeta potential values.	Determine the Zeta potential values	K3
5.2	Process at electrodes-Butler-Volmer equation-high and low field approximation-Tafel equation	Deduce the Butler-Volmer and Tafel equation	K4
		Calculate anodic and cathodic current	K4
5.3	Electrochemical corrosion of metals, constructions and use of Pourbaix and Evans Diagrams and prevention of corrosion.	Write the uses of Pourbaix and Evans Diagram	K3
		Summarize the different methods of corrosion prevention	K2

4.Mapping Scheme for the PO, PSOs and Cos

L-Low M-Moderate H- High

Course Title: THERMODYNAMICS AND ELECTROCHEMISTRY
Course Code: P19CH307

	PO 1	**PO 2**	**PO 3**	**PO 4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PSO1**	**PSO2**	**PSO3**	**PSO4**
CO1	H	H	L	-	-	-	-	-	-	M	-	H	M
CO2	M	H	-	-	-	-	-	-	-	M	-	L	M
CO3	M	H		-	-	-	-	-	-	L	-	H	L
CO4	L	-	L	M	M	-	-	-	-	M	-	-	-
CO5	-	L	M	L	-	-	-	-	-	H	-	M	L
CO6	H	L	-	-	L	-	-	-	-	-	-	L	-

5.Course Assessment Methods

DIRECT:

1. Continuous Assessment Test (Model Exams) I, II
2. Open book test; Cooperative learning report, Assignment; Journal paper review, Group Presentation, Project report, Poster preparation, Proto-type or Product Demonstration etc. (as applicable)
3. End Semester Practical Examination

INDIRECT:

1. Course-end survey

Xxxx- Revised content

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ELECTIVE COURSE: II - BIO-INORGANIC CHEMISTRY

SEMESTER : III **CODE : P19CH3:2**
CREDITS : 4 **TOTAL HOURS : 75**
Hours /week:5

1.Course Outcomes

After the successful completion of this course the students will be able to

S.No.	Course Outcomes	Level	Unit
1	Explain the role of metal complexes, alkali and alkaline earth metals in living systems	K5	I
2	Illustrate various membrane transport mechanisms in biological systems	K4	II
3	Categorize metalloproteins as redox agents and oxygen carriers based on their structure and functions	K4	III
4	Justify the role of various metalloproteins in photosynthesis	K5	III
5	Summarize the physiological and biochemical functions of minerals and their toxicity	K5	IV
6	Correlate the structure and mode of action of therapeutic drugs	K4	V

2A. Syllabus

UNIT-I **MEALS IN BIOLOGY** **15Hours**

Hours

1.1 An overview of metals in Biology - Essential metals –their fate and conversion in Biological systems. Bio- organometallic chemistry – Metal ion Complexation – Thermodynamics and Kinetics – Electron transfer reactions.

1.2 Biological role of alkali metals - Alkali and alkaline earth metals complexes: Complexes of β-diketone, crown ethers, cryptands and spiranes; Template Effect, macro-cyclic effect , macro- cyclic effect.

UNIT-II **TRANSPORT OF METALS** **15 Hours**

Structure, characteristics and composition of cell membrane- The fluid model - Membrane Transport: Active and passive transport, Ping-Pong model of facilitated diffusion- Iono-phores, Transporter proteins- Ion pumps – Mechanism of Na^+ and K^+ pumps- Gated transport -voltage gated transport. Types of ports in ion transport – uniport- symport – Antiport. Gap Junctions

Xxxx- Revised content

UNIT – III Metalloproteins 15 Hours

3.1 Bio-Redox agents: Fe-S proteins-Ferredoxin and Rubredoxin, HIPIPs-Functions and Structure , Non-heme iron proteins (Ferritin, Hemosiderin)

3.2 Metals as Carriers - Iron Containig Oxygen Carriers –Myoglobin – Hemoglobin – Structure and Prosthetic group –Mechanism of reversible binding of dioxygen and Cooperativity –CO binding to Fe and model Complexes containing Cobalt.- Structure and Function of Vitamin-B_{12}

3.3 Oxygen uptake proteins: Cytochrome P-450 enzyme.

3.4 Photosynthesis- Light phase and dark phase reactions, Photosystem I and II. Nitrogen Fixation- Invivo Copper proteins: Blue copper proteins(Cupredoxins)-Type I-Plastocyanin - Type III-Hemocyanin. Non blue copper proteins-Type II-Galactoseoxidase and Superoxidase dimutase .Some other copper protein -Ceruloplasmin.

UNIT- IV METAL DIETARY REQUIREMENT AND TOXICITY 15 Hours

Minerals in Diet – Requirement of various minerals in Physiological and biochemical functions-Classification of minerals according to their functions in the body – Digestion and Absorption ofminerals – Mechanism of Iron Absorption – Ferroprotein secretion.

4.2 Toxicity Due to Metals - Bio-chemistry of toxic Metals Pb, Cd, Hg, Al, Fe, Cu, Pu -Detoxification by metal chelates.

UNIT–V METALS IN MEDICINE 15Hours

Structure, Mode of action, Bio – availability and solubility and advantages and side effects ofthe following drugs:

5. 1. Cancer therapy: Cis-platin and its mode of action.
5. 2. Radiotherapy: Radio-pharmaceuticals- Technetium. Chemotherapy – basics and applications
5.3. Anti-rheumatic agents: Gold containing drugs and their action.
5.4. Psychopharmacological drugs: Lithium drugs and their mode of action.
5.5. Contrast enhancing agents for MRI: MRI imaging, Synthesis of Gadolinium based contrast agents.

Xxxx- Revised content

2B.Topics for Self-Study:

S.No.	Topics	Web Links
1	Alkali metals in biology	https://link.springer.com/referenceworkentry/10.1007/978-3-319-39193-9_154-1
2	Ions transport	https://www.intechopen.com/books/ion-channels-in-health-and-sickness/introductory-chapter-ion-channels
3	oxygen uptake	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2554684/pdf/bullwho00238-0086.pdf https://www.sciencedirect.com/science/article/abs/pii/S1380732301800029
4	Detoxification method	https://www.scribd.com/read/149973523/A-Textbook-on-EDTA-Chelation-Therapy-Second-Edition#
5	Metals in medicine	https://www.researchgate.net/publication/230812100_Metals_in_Medicine

2C.Text Books:

1. Asim K. Das. "Bio-Inorganic chemistry", Books and Allied Publishers, 2007. **(Unit I-IV)**
2. Subbiah Balaji, "Nanobiotechnology", MJP Publishers, Chennai, 2010. **(Unit -V)**

2D.Recommended Reference Books:

1. Stephen J. Lippard, Jeremy Mark Berg, "Principles of Bioinorganic Chemistry", University Science Books, 1994.
2. James E. Dabrowiak, "Metals in Medicine (Inorganic Chemistry: A text book series)", Willey Black well, 2017.K.J. Laidler, "Chemical Kinetics", Tata McGraw-Hill, New Delhi, 2003.

3.Specific Learning Outcomes (SLO)

Unit/ Section	Course Content	Learning outcomes	Blooms Taxonomy Level of Transaction
I	**MEALS IN BIOLOGY**		
	An overview of metals in Biology - Essential metals – their fate and conversion in Biological systems. Bio-organometallic chemistry - Metal ion Complexation - Thermodynamics and Kinetics - Electron transfer reactions.	Inspect the role of metal complexes in living systems.	K5

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	Biological role of alkali metals - Alkali and alkaline earth metals complexes: Complexes of β-diketone, crown ethers, cryptands and spiranes; Template Effect, macro-cyclic effect, macro-cyclic effect.	Distinguish the role of alkali metals, alkaline earth metals and organometallic compounds in biological systems.	K5
UNIT-II **TRANSPORT OF METALS**			
2.1	Structure, characteristics and composition of cell membrane- The fluid model - Membrane Transport: Active and passive transport, Ping-Pong model of facilitated diffusion- Ionophores, Transporter proteins- Ion pumps – Mechanism of Na$^+$ and K $^+$ pumps- Gated transport -voltage gated transport.	Examine the different mechanismsof membrane transport in biological systems.	K4
2.2	Types of ports in ion transport – uniport- symport – Antiport. Gap Junctions.		K4
Unit - III	**METALLOPROTEINS**		
3.1	Bio-Redox agents: Fe-S proteins- Ferredoxin and Rubredoxin, HIPIPs-Functions and Structure, Non-heme iron proteins (Ferritin, Hemosiderin)	Inspect the role of biomolecules that act as redox agents with relation to their structure.	K4
3.2	Metals as Carriers - Iron Containing Oxygen Carriers – Myoglobin – Hemoglobin – Structure and Prosthetic group – Mechanism of reversible binding of dioxygen and Cooperativity – CO binding to Fe and model Complexes containing Cobalt - Structure and Function of Vitamin-B$_{12}$.	Distinguish the metal complexesthat act as oxygen carriers based on their structure and functions	K4
3.3	Oxygen uptake proteins: Cytochrome P-450 enzyme	Justify the significance of Cyt-450.	K5
3.4	Photosynthesis- Light phase and dark phase reactions, Photosystem I and II. Nitrogen Fixation- Invivo Copperproteins: Blue-copper proteins	Distinguish the light and dark phase reactions and the functions of blue copper proteins and non-blue copper proteins.	K5

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	(Cupredoxins) - Type I - Plastocyanin -Type III - Hemocyanin. Non-blue copper proteins- Type II - Galactose oxidase and Superoxidedismutase. Some other copper protein - Ceruloplasmin.		
Unit - 4	**METAL DIETARY REQUIREMENT AND TOXICITY**		
4.1	Minerals in Diet – Requirementof various minerals in Physiological and biochemical functions - Classification of minerals according to theirfunctions in the body – Digestion and Absorption of minerals –Mechanism of Iron Absorption – Ferroprotein secretion.	Perceive the requirement of various minerals and their digestion and absorption by the human body.	K5
4.2	**Toxicity Due to Metals -** Bio-chemistry of toxic Metals Pb, Cd, Hg, Al, Fe, Cu, Pu - Detoxification by metal chelates.	Evaluate the toxicity and detoxification effect of metals and metal chelates respectively.	K5
Unit - 5	**METAL DIETARY REQUIREMENT AND TOXICITY**		
5.1	Cancer therapy: Cisplatin and its mode of action.	Differentiate the various chemotherapeutic drugs as Anti-Cancer agents, Anti-rheumaticagents, Psychopharmacological drugs and Contrast enhancing agents and correlate their structure with the mode of action.	K3
5.2	Radiotherapy: Radio-pharmaceuticals- Technetium. Chemotherapy – basics and applications		K3
5.3	Anti-rheumatic agents: Gold containing drugs and their action.		K3
5.4	Psychopharmacological drugs: Lithium drugs and their mode of action.		K3
5.5	Contrast enhancing agents for MRI: MRI imaging, Synthesis of Gadolinium based contrast agents.		K3

Xxxx- Revised content

4.Mapping Scheme for COs, POs and PSOs

L-Low **M-Moderate** **H- High**

Course Title: BIO-INORGANIC CHEMISTRY
Course Code: P19CH3:2

Mapping	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PSO1	PSO2	PSO3	PSO4
CO1	M	M	M	L	M	-	-	-	-	M	L	M	-
CO2	M	L	M	H	M	-	-	-	-	H	M	L	L
CO3	H	H	M	M	H	-	-	-	-	M	H	M	L
CO4	M	M	M	-	H	-	-	-	-	H	M	-	L
CO5	L	M	L	M	M	-	-	H	-	M	L	H	-
CO6	H	M	M	H	H	-	-	H	-	H	L	L	H

5.Course Assessment Methods

Direct

1. Continuous Assessment Test (Model Exams) I,II
2. Open book test; Cooperative learning report, Assignment; Journal paper review, Group Presentation, Project report, Poster preparation, Proto-type or Product Demonstration etc. (as applicable)
3. End Semester Practical Examination

Indirect

1. Course-end survey

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Xxxx- Revised content

Xxxx- Revised content

Core Practical: V

PHYSICAL CHEMISTRY PRACTICAL (NON ELECTRICAL)

(Lab. Cum Theory)

Semester : I1I **Code : P19CH3P5**
Credits : 3 **Total Hrs :90**
Hours/week:6

1.Course Outcomes:

At the end of this course, the students will be able to

S.No.	Course Outcomes	Level
1	Determine the Arrhenius parameters from kinetics data	K5
2	Evaluate the influence of ionic strength on rate constant	K5
3	Recommend the optimal conditions to automotive antifreeze using colligative properties	K5
4	Choose specific and selective adsorbents for industrial and environment related problems using Adsorption isotherms	K5
5	Measure qualitative and quantitative parameters of components in drugs, cosmetics, food and beverages, polarimetrically	K5
6	Assess the heat of solution for solute and solvent in a given mixture	K5

2A. Syllabus

NON-ELECTRICAL EXPERIMENTS:

1. Comparison of strength of acids by the study of kinetics of hydrolysis of an ester.
2. Evaluation of E_a and A by studying the kinetics of acid catalysed hydrolysis of ethyl acetate.
3. Determination of molecular weight by Rast method.
4. Construction of phase diagram of a congruent system.
5. Determination of critical solution temperature of phenol-water system and study of the effect of NaCl on miscibility temperature.
6. Comparison of the strength of acids by the kinetic study of iodination of acetone.
7. Effect of an inert salt on the kinetics of clock reaction between I^- and $S_2O_3^{2-}$.
8. Construction of adsorption isotherm for the adsorption of oxalic acid and charcoal.
9. Polarimetric study of the kinetics of acid catalysed inversion of sucrose.
10. Determination of heat of solution of a substance (benzoic acid or ammonium oxalate) by the measurement of its solubility as a function of temperature.

2B.Text Books:

1. J.N.Gurthu and R.Kapoor, “Advanced Experimental Chemistry”, S. Chand and Co., 1987.
2. Sundaram, Krishnan, Raghavan, “Practical Chemistry (Part II)”, S.Viswanathan and Co.Pvt. Ltd., 1996.

2C.Reference Books:

1. David P. Shoemaker, Carl W. Garland and Joseph W. Nibler, “Experiments in Physical Chemistry”, 5th Edition, McGraw- Hill Book company, 1989.

3.Specific Learning Outcomes (SLO)

Unit	Course Content	Learning Outcomes	Blooms Taxonomic levels of Transaction
1.1	• Comparison of strength of acids by the study of kinetics of hydrolysis of an ester • Evaluation of E_a and A by studying the kinetics of acid catalysed hydrolysis of ethyl acetate • Comparison of the strength of acids by the kinetic study of iodination of acetone • Effect of an inert salt on the kinetics of clock reaction between I^- and $S_2O_3^{2-}$.	Determine the rate, order, molecularity and frequency factor of the given reaction.	K5
		Explain the influence of ionic strength on rate constant	K5
		Justify the charge of the active species involved in the reaction.	K5
		Evaluate the acid strength by following the kinetics of Iodination of acetone.	K5
	• Determination of molecular weight by Rast method.	Illustrate the colligative properties.	K5
		Determine the molal depression constant (K_f) of a given solvent.	K5
		Determine the transition temperature of given salt hydrate.	K5
		Estimate the molecular weight of unknown compound	K5
	• Construction of phase diagram of a congruent system • Determination of critical solution temperature of phenol-water systemand study of the effect of NaCl on miscibility temperature	Determine the congruent melting point by constructing the phase diagram.	K5
		Evaluate the critical solution temperature of partially miscible liquid systems.	K5

		Evaluate the effect of impurities on CST.	K5
	- Construction of adsorption isotherm for the adsorption of oxalic acid and charcoal.	Explain the factors affecting surface reactions	K5
		Compare physisorption and chemisorption	K5
		Choose the suitable adsorption isotherms to predict thekinetics	K5
	- Polarimetric study of the kinetics of acid catalysed inversion of sucrose	Explain the mechanism of inversion of sugar	K5
		Evaluate the kinetic parameter of chemical reactions by polarimetry.	K5
	- Determination of heat of solution of a substance (benzoic acid or ammonium oxalate) by the measurement of its solubility as a function of temperature.	Evaluate the heat of solution.	K5
		Predict the feasibility of the reaction from the thermodynamic data	K5

4.Mapping of POs, PSOs and Cos

H- High; M- Moderate; L- Low

Course Title: PHYSICAL CHEMISTRY PRACTICAL (NON ELECTRICAL)
Course Code : P19CH3P5

Mapping	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PSO1	PSO2	PSO3	PSO4
CO1	H	H	M	M	H	--	M	H	--	H	H	H	M
CO2	H	H	M	M	H	--	M	H	--	H	H	H	H
CO3	H	H	H	H	H	--	H	H	--	H	H	H	M
CO4	H	H	H	H	H	--	H	H	--	H	H	H	M
CO5	H	H	H	H	H	--	H	H	--	H	H	H	M
CO6	H	H	L	M	H	--	M	H	--	H	H	H	M

5.COURSE ASSESSMENT METHODS

Direct
1. Continuous Internal Assessment 2. Model Exam 1 & 2 3. Viva -Voce 4. End Semester Examination
Indirect
1. Course-end survey

Core Practical: VI

PHYSICAL CHEMISTRY PRACTICAL (Electrical)

Semester : III **Code : P19CH3P6**
Credits : 3 **Total Hrs :90**
Hours/week:6

1.Course Outcomes:

At the end of this course, the students will be able to:

S.No.	Course Outcomes	Level
1	Utilize the potentiometer and conductivity meter to estimate the strength of various acids, bases, halides and other salts in the given mixtures	K3
2	Compare the reliability of results for a given experiment by Conductometric and Potentiometric methods	K5
3	Construct different types of electrochemical cells	K6
4	Prioritize the methods of analysis for an experiment in a given set of conditions	K5
5	Analyse the solubility product of the given salt by conductometric and potentiometric methods	K4

2A. Syllabus

ELECTRICAL EXPERIMENTS:

1. Conductometric determination of dissociation constant of a weak acid.
2. Potentiometric determination of pK_a of an acid.
3. Measurement of single electrode potentials of Zn^{2+} / Zn and Cu^{2+}/Cu electrodes.
4. Potentiometric redox titration of $KMnO_4$ with KI or Fe^{2+} or Ce^{4+} and determination of standard redox potential.
5. Potentiometric estimation of mixture of halides.
6. Conductometric estimation of mixture of halides
7. Conductometric estimation of the components of buffer.
8. Conductometric estimation of mixture of weak and strong acids.
9. Conductometric precipitation titration of $BaCl_2$ with $MgSO_4$ and K_2SO_4.
10. Conductometric titration of NH_4Cl and HCl against NaOH.
11. Conductometric titration of mixture of alkali against HCl.
12. Determination of solubility product by
    a) Conductometric method b) Potentiometry - Concentration cell method
    c) Potentiometry - Chemical cell method.
13. Potentiometric estimation of mixture of weak and strong acids.

14. Conductometric study of the kinetics of saponification of ester- (Internal/ Demonstration only)

2B.Text Books:

1. J.N. Gurthu and R. Kapoor, "Advanced Experimental Chemistry", S. Chand and Co.,1987.
2. Sundaram, Krishnan, Raghavan, "Practical Chemistry (Part II)", S.Viswanathan and Co.Pvt.,1996.

2C.Reference Books:

1. David P.Shoemaker, Carl W.Garland and Joseph W.Nibler, "Experiments in Physical Chemistry", 5th Edition, McGraw- Hill Book company, 1989.

3.Specific Learning Outcomes (SLO)

S. No	**Course Content**	**Learning Outcomes**	**Blooms Taxonomic level of Transaction**
1	Conductometric determination of dissociation constant of a weak acid.	Examine the dissociation constant of weak acids by conductometric method.	K3
2	Potentiometric determination of pK_a of an acid.	Determine the dissociation constant of weak acids by potentiometric method.	K3
3	Measurement of single electrode potentials of Zn^{2+}/Zn and Cu^{2+}/Cu electrode	Measure electrode potentials of various electrodes	K6
4	Potentiometric redox titration of $KMnO_4$ with KI or Fe^{2+} or Ce^{4+} and determination of standard redox potential.	Interpret potentiometric redox titrations for the estimation of the given analyte.	K5
5	Potentiometric estimation of mixture of halides.	Estimate the mixture of halides by potentiometry.	K4
6	Conductometric estimation of mixture of halides	Estimate mixture of halides by conductometric method.	K4

7	Conductometric estimation of the components of buffer	Estimate the amount of different components in buffer mixtures.	K4
8	Conductometric estimation of mixture of weak and strong acids	Evaluate the concentration of mixture of acids by conductometric method.	K5
9	Conductometric precipitation titration of $BaCl_2$ with $MgSO_4$ and K_2SO_4	Interpret conductometric precipitation titration for the estimation the given analyte.	K5
10	Conductometric titration of NH_4Cl and HCl against NaOH.	Estimate the NH_4Cl and HCl present in a mixture conductometrically.	K4
11	Conductometric titration of mixture of alkali against HCl	Estimate the components present in a mixture of bases by conductometric method	K4
12	Determination of solubility product by a) Conductometric method b) Potentiometry - Concentration cell method c) Potentiometry - Chemical cell method.	Evaluate the solubility product of sparingly soluble salts by conductometric and potentiometric method	K5
13	Potentiometric estimation of mixture of weak and strong acids	Estimate the components of mixture of weak and strong acids by potentiometric method	K4
14	Conductometric study of the kinetics of saponification of ester- (Internal/ Demonstration only)	Identify the order of saponification of ester by following the kinetics conductometrically.	K2

Mapping Scheme for the PO, PSOs and Cos

L-Low M-Moderate H- High

Course Title: PHYSICAL CHEMISTRY PRACTICAL (Electrical)

Course Code : P19CH3P6

Mapping	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PSO1**	**PSO2**	**PSO3**	**PSO4**
CO1	H	H	H	H	M	L	-	-	-	H	M	M	H
CO2	H	H	M	H	H	L	L	-	-	H	H	H	H
CO3	H	H	H	M	M	-	-	L	L	H	M	L	H
CO4	H	H	M	H	H	-	L	M	M	H	M	L	M
CO5	M	H	-	H	H	L	-	-	-	M	H	-	H
CO6	M	H	M	M	H	M	L	-	L	H	M	M	L

5.Course Assessment Methods

Direct
1. Continuous Internal Assessment 2. Model Exam 1 & 2 3. Viva -Voce 4. End Semester Examination
Indirect
1. Course-end survey

Xxxx- Revised content

PRACTICAL PREPARATORY COURSE – III

SEMESTER: III **TOTAL HOURS: 30**

CODE: P19CH3P5& P19CH3P6

COURSE OBJECTIVES:

- To learn the concepts of Physical Chemistry experiments in P19CH3P5& P19CH3P6.
- To understand the principle and methodology behind various techniques.
- To learn the laboratory precautions, procedures and preparations involved in the experiments.

UNIT-I

Concentration Units-Mole concept, normality, molarity, molality, mole fraction, weight %, volume %, ppm, ppb-Types of solutions-primary and secondary standard substances-standard solutions- dilution formula- Calculations- Graphs – Regression coefficient-Slope and intercept.

Chemical kinetics- Reaction rates-Reaction molecularities -order of a reaction-Determination of the order of a reaction-Graphical method- Arrhenius equation - The temperature co-efficient-Temperature control using Thermostat.

Oscillatory reactions: Principle of Iodination of acetone- - Clock reaction-influence of ionic strength on rate constant.

UNIT-II

Polarimetry - optical rotation -mechanism of inversion of cane sugar.
Thermo chemistry-Heat of formation-Heat of combustion-Heat of solution –integral heat of dilution-heat of hydration. Use of indicators in titrations.

Colligative properties and Phase equilibria - Phase-Component-degree of freedom-Reduced Gibbs phase rule-eutectic temperature-eutectic composition-freezing point diagram of binary mixtures- examples of one, two and three component systems.

Surface phenomenon – differences between adsorption and absorption - adsorbent-adsorbate-Physisorptions-chemisorption-types of adsorption isotherms (Only final equations).

UNIT-III

Electrochemistry-Electrical conductance of electrolytes-Specific conductivity-Equivalent conductivity-Molar conductivity- conductance value of ions-Effect of dilution on conductivity.
Ostwald's dilution law-Debye-Huckel Onsager equation- Debye –Huckel limiting law-Kohlrausch law (Only final equation).

Conductometric titrations-Principle & types, Standardisation of conductometer-Wheatstone's meter bridge-Conductivity cell-Advantages of conductometric titrations.
Concept of solubility- Solubility Product – Common ion effect - pH scale – Buffer.

Potentiometric titrations- Galvanic cell- Nernst Equation - Electrode potential- Electrochemical series-Types of electrodes- salt bridge- liquid junction potential- standardization of potentiometer- Standard cell and Western cell.

Xxxx- Revised content

Measurement of EMF of cell-overall cell reactions- writing cell diagram- Applications of potentiometric titrations.

TEXT BOOKS:

1. Jagadamba singh, R.K.P. Singh, Jaya Singh, LDS Yadav, I.R. Siddiqui and Jaya Shrivastava, "Advanced Practical Chemistry" Pragati Prakasham Publishers, Fifth Edition, 2014.
2. B.Viswanathan and P.S. Raghavan, "Practical Physical Chemistry" Viva Books Pvt. Ltd., 2006. **(Unit I-III)**

REFERENCES:

1. B. Yadav, "Advanced Practial Physical Chemistry" Satyendra Rastogi Mitra, 34th Edition, 2014.
2. David P. Shoemaker, Carl-W.Garland and Joseph W. Nibler, Experiments in Physical Chemistry, Mc Graw-Hill-International, Fifth Edition, 2004.

COMPONENTS FOR EVALUATION

Test -1	**Max marks :30 (Part A 2 X 10, Part B 2 x5)**
Test – 2	**Max marks :30 (Part A 2 X 10, Part B 2 x5)**

Xxxx- Revised content

PROJECT PREPARATORY COURSE

SEMESTER : III **CODE : P19CH4PJ**
TOTAL HOURS: 15

COURSE OBJECTIVES:

- To learn the fundamentals of Short term research Projects
- To understand the basic requirements of a project work and plan ahead of the project work.

UNIT- I RESEARCH METHODOLOGY

Basic elements of Research – Objectives – Types of research – Steps involved in research – Identifying a PROBLEM for project- Evolving strategies for solving – Designing feasible experiments – planning and scheduling a Project

UNIT- II REVIEW OF LITERATURE

Sources of literature- primary – secondary – tertiary – importance and characters of Monographs, Journals, Notes and Communications. Methods of literature survey – Chemical Abstracts and Indexing – Computer aided searches – Use of Search engines and advanced searches using Google Scholar , Scifinder– PubMed , RSC, PDB. Ordering and scheming the literature review – Identification of gaps in literature

UNIT- III PREPARATION OF A PROJECT REPORT AND PRESENTATION

Planning a project report – criteria for selection of the titles and subtitles –Scientific language for writing – Tenses and voices for the Introduction – Review and Report. Language editors and raters and their usage- Bibliography preparation – styles and types – Methods of including references in MsWord – Mendeleev and Microsoft End note for reference. Simple tips for usage of MS word, Excel, power point, Origin and OneNote for project report preparation

REFERENCES:

1. Research and Writing across the disciplines - P Ramadass and A. Wilson Aruni , MJP Publishers, Chennai, 2009.
2. https://www.mendeley.com/download-mendeley-desktop/
3. http://cassi.cas.org/
4. https://www.cas.org/

COMPONENTS FOR EVALUATION:

Test -1 **Max marks :30 (Part - A: 2 X 10, Part – B: 2 x5)**

Test – 2 **Max marks :30 (Part – A: 2 X 10, Part – B: 2 x5)**

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Core Course: VIII **INORGANIC SPECTROSCOPY**

Semester : IV **Code : P19CH408**
Credits: 5 **Total Hrs: 90**
Hours/week:6

1.Course Outcomes

After the successful completion of this course the students will be able to

S.No.	Course Outcomes	Level	Unit
1	Explain the metal-ligand interaction in transition metal complexes through electronic spectra	K5	I
2	Justify the structure and bonding of coordination compounds using IR and Raman Spectroscopy	K5	II
3	Analyze the splitting pattern of NMR signals with respect to different nuclei present in inorganic compounds.	K4	III
4	Analyze the EPR spectra of Inorganic compounds based on the effect of spin-orbit coupling and crystal field effects.	K4	IV
5	Examine the effect of magnetic and quadrupole fields on Mossbauer spectra of simple Molecules.	K4	V
6	Deduce the structure of coordination compounds using data derived from Electronic, IR, Raman, NMR, ESR and Mossbauer spectroscopic techniques.	K5	V

2A. Syllabus

UNIT- I ELECTRONIC SPECTROSCOPY 18 HOURS

Electronic Spectroscopy of complexes- characteristics of d-d transitions, selection rules for d-d transitions- Term symbols for d – ions, Use of Orgel diagrams for d^{1-10} octahedral and tetrahedral complexes, Tanabe-Sugano diagrams for $d^1$and d^6 octahedral complexes only. Effect of Jahn -Teller distortion and spin - orbit coupling on spectra. Charge transfer spectra (LMCT and MLCT)- Intensity of Charge transfer transitions in inorganic and coordination compounds , Electronic absorption spectra of low spin and strong field complexes.

UNIT- II IR AND RAMAN SPECTROSCOPY 18 HOURS

Combined uses of IR and Raman Spectroscopy in the structural elucidation of simple molecules like H_2O, ClF_3 NO_3^{-}, and ClO_3^-. Effect of Co-ordination on ligand vibrations – uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate,

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sulphate and dimethyl sulphoxide. Effect of isotopic substitution on the vibrational spectra of

Xxxx- Revised content

molecules. Differentiation of coordinated water and lattice water. Applications of IR to identify terminal and bridging carbonyl group.

UNIT- III NMR SPECTROSCOPY 18 HOURS

Applications of NMR to inorganic compounds-(spin-spin coupling involving different nuclei ^{1}H,^{31}P,^{13}C) NMR of metal hydrides(H^{1} NMR)- Metal carbonyls(C^{13} NMR)- F^{19}, P^{31} NMR. Effect of quadrupolar nuclei (^{2}H,^{10}B,^{11}B) on the ^{1}H NMR spectrum. NMR of paramagnetic molecules – isotopic shifts, contact and Pseudo-contact interactions- lanthanide shift reagents.

UNIT- IV EPR SPECTROSCOPY 18 HOURS

Basic principle – characteristics of 'g' –Hyperfine splitting –selection rules – factors affecting the magnitude of the 'g' values. 'g' value of transition metal ions –dependence on spin – orbit coupling and crystal field effects. EPR of d^{1} to d^{9} systems of first transition series. Tetragonally distorted copper complexes – Zero-field splitting and Kramer's degeneracy. Solid state EPR – spin-lattice relaxation – spin-spin relaxation – exchange processes.

UNIT-V Magneto-chemistry & Mossbauer Spectroscopy 18 HOURS

5.1 Magneto-chemistry

Determination of magnetic susceptibility by Guoy and Faraday methods. Magnetic properties of low spin and high spin octahedral complexes of first row transition metals- Curies law, Curies-Weiss law, Curie temperature and Neel temperature, Types of Magnetism- Paramagnetism, Diamagnetism, Ferro and anti-ferromagnetism.

5.2 Mossbauer Spectroscopy:

Principle- Doppler effect –Recoil energy- isomer shift – quadrupole effect – magnetic interactions - magnetic field on spectra –simple applications to iron and tin compounds.

2B.Topics for Self-Study:

S.No	Topics	Web link
1	Microstates in electronic spectroscopy	https://www.youtube.com/watch?v=oUm493PIPJA
2	Transition Metal Cyclopentadienyl Nitrosyl Complexes	https://www.youtube.com/watch?v=52oh47-Kti4
3	Fluxional behavior in NMR spectroscopy	https://www.youtube.com/watch?v=teXjVQM2fsw
4	Spin orbit coupling	https://www.youtube.com/watch?v=Np6KRP-tl-o&pbjreload=101
5	Mossbauer spectrum- spin cross over & Zeeman splitting	https://www.youtube.com/watch?v=pbMNfO-Z5iA

2C.Text Book(s):

1. B.K. Sharma, “Spectroscopy”, Krishna Prakashan, New Delhi, 1993. **(Unit I-V)**
2. P.S. Sindhu, “Molecular Spectroscopy” Tata McGraw Hill, 2000.
3. H. Kaur, “Spectroscopy” Pragati Publications, Meerut, 2001.
4. V.B.Pathania, “Spectroscopy” Campus Books, New Delhi, 2002

2D.Reference Books:

1. R. S. Drago, “Physical Methods in Inorganic Chemistry”, East West Publishers, New Delhi, 1965.
2. EAV Ebsworth, “Structural Methods in Inorganic Chemistry”, ELBS, Oxford,1988.
3. A. Abdul Jameel “Application of Physical Methods to Inorganic compounds” JAN Publication, Trichy, 2003.
4. James E. Huheey, Ellen A Keiter and Richard L. Keiter, “Inorganic Chemistry: Principles of Structure and Reactivity”, Pearson Education, India, 2014.

3.Specific Learning Outcomes (SLO)

Unit	Course Content	Learning Outcomes	Blooms Taxonomic Levels of Transaction
	Unit- I ELECTRONIC SPECTROSCOPY		
1	Electronic Spectroscopy of complexes - characteristics ofd-d transitions - selection rules for d-d transitions	Identify the types and the rules governing the transitions in d-block elements	K3
	Term symbols for d – ions	Categorize the term symbols of various microstates in d-block ions	K4
	Use of Orgel diagrams for d^{1-10} octahedral and tetrahedral complexes	Analyze the relative energies of electronic terms in transition metal complexes	K4
	Tanabe-Sugano diagrams for d^1 and d^6 octahedral complexes only	Explain the absorptions in the electronic spectra of coordination compounds	K5
	Effect of Jahn -Teller distortion and spin - orbit coupling on spectra	Examine the effect of Jahn -Teller distortion and spin - orbit coupling on the electronic transitions	K4
	Charge transfer spectra(LMCT and MLCT) - Intensity of Charge transfer transitions in inorganic and coordination compounds	Examine the interaction between MOs of metal and ligand in excited state	K4
	Electronic absorption spectra of low spin and strong field complexes	Compare the absorption spectra of low spin, strong field complexes	K4
	Unit- II IR AND RAMAN SPECTROSCOPY		
2	Combined uses of IR and Raman Spectroscopy in the structural elucidation of simple molecules like H_2O, ClF_3, NO_3^- and ClO_3^-	Categorize the structure of simple molecules using IR and Raman spectroscopy	K4

	Effect of Co-ordination on ligand vibrations	Analyze the effect of coordination of the ligand stretching frequencies	K4
	Uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulphoxide	Deduct the structure of metal complexes containing differenttypes of ligands	K5
	Effect of isotopic substitution on the vibrational spectra of molecules	Assess the effect of isotopic substitution	K5
	Differentiation of coordinated water and lattice water	Distinguish coordinated and lattice water molecules	K4
	Applications of IR to identify terminal and bridging carbonyl group	Compare the vibrational frequencies of coordinate carbonyl group using IR	K5
	Unit- III NMR SPECTROSCOPY		
3	Applications of NMR to inorganic compounds-(spin-spin coupling involving different nuclei ^{1}H, ^{31}P, ^{13}C)	Classify the spin-spin coupling among various nuclei in inorganic compounds	K4
	NMR of metal hydrides (H^{1} NMR), Metal carbonyls (C^{13} NMR), F^{19}, P^{31} NMR	Analyze the NMR of different nuclei in inorganic compounds	K4
	Effect of quadrupolar nuclei (^{2}H,^{10}B,^{11}B) on the ^{1}H NMR spectrum	Categorize the splitting pattern by coupling with quadrupolar nuclei	K4
	NMR of paramagnetic molecules - isotopic shifts, contact and Pseudo-contact interactions- lanthanide shift reagents	Examine the NMR of paramagnetic compounds	K4
	Unit- IV EPR SPECTROSCOPY		
4	EPR Spectroscopy - Basic principle - characteristics of ‘g’	Analyze the interaction between magnetic moments of nucleus and	K4

	- Hyperfine splitting - selection rules	electrons in atoms and the rules governing it	
	Factors affecting the magnitude of the ‘g’ values -‘g’ value of transition metal ions - dependence on spin – orbit coupling and crystal field effects	Examine the effect of spin orbit coupling and crystal field effects on the magnitude of g value in ions of d-block	K4
	EPR of d^1 to d^9 systems of first transition series	Categorize the EPR of 1st row d-block compounds	K4
	Tetragonally distorted copper complexes	Inspect the effect of tetragonal distortion (elongation) in octahedral copper complexes	K4
	Zero-field splitting and Kramer’s degeneracy	Analyze the effect of magnetic field on EPR spectra	K4
	Solid state EPR - spin-lattice relaxation – spin-spin relaxation – exchange processes	Examine the effect of relaxation process on EPR spectra	K4
	Unit- V Magneto-chemistry & Mossbauer Spectroscopy		
	Magneto-chemistry - Determination of magnetic susceptibility by Guoy and Faraday methods	Apply of the different methods to determine magnetic susceptibility	K3
	Magnetic properties of low spin and high spin octahedral complexes of first rowtransition metals	Analyze the magnetic properties of 1st row d-block elements	K4
	Curies law, Curies-Weiss law, Curie temperature and Neel temperature	Illustrate the effect of magnetization in a paramagnetic material	K2
	Types of Magnetism-Paramagnetism, Diamagnetism, Ferro and anti-ferromagnetism	Outline the different types of magnetism and their characteristics	K2
5.2	**Mossbauer Spectroscopy** – Principle - Doppler effect – Recoil energy- isomer shift –	Examine the basic principles and effects of Mossbauer spectroscopy	K4

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	quadrupole effect		
	Magnetic interactions - magnetic field on spectra	Explain the effect of magnetic field on spectra	K2
	Simple applications to iron and tin compounds	Apply the principles of Mossbauer spectroscopy to iron and tin compounds	K3

4.Mapping of COs with POs and PSOs

L-Low **M-Moderate** **H- High**

Course Tittle: INORGANIC SPECTROSCOPY **Course Code:P19CH408**													
	PO 1	**PO 2**	**PO 3**	**PO 4**	**PO 5**	**PO 6**	**PO 7**	**PO 8**	**PO 9**	**PSO 1**	**PSO 2**	**PSO 3**	**PSO 4**
CO1	H	H	-M	H	M	-	L	-	-	H	-	M	M
CO2	H	H	L	M	M	L	H	L	M	H	H	M	H
CO3	H	H	L	M	M	L	H	L	M	H	H	M	H
CO4	H	M	L	L	L	L	M	-	L	M	M	L	M
CO5	H	L	L	L	L	-	L	-	L	L	-	-	L
CO6	H	M	M	M	M	M	H	L	M	-	M	M	H

5.Course Assessment Methods

Direct

1. Continuous Assessment Test (Model Exams) I,II
2. Open book test; Cooperative learning report, Assignment; Journal paper review, Group Presentation, Project report, Poster preparation, Proto-type or Product Demonstration etc. (as applicable)
3. End Semester Practical Examination

Indirect

1. Course-end survey

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CORE COURSE : IX - GROUP THEORY & SPECTROSCOPY

SEMESTER : IV **CODE : P19CH409**
CREDITS : 5 **TOTAL HOURS : 90**
Hours /week:6

1.Course Outcomes:

After the successful completion of this course, the students will be able to:

S.No.	Course Outcomes	Level	Unit
1.	Categorize the molecules based on symmetry elements, symmetry operations and point groups	K4	I
2.	Evaluate the selection rules for spectroscopy and hybridization schemes using the concept of molecular symmetry	K5	II
3.	Explain the principles involved in different spectroscopic techniques	K2	III
4.	Interpret the structure of molecules based on IR and Raman spectroscopy	K5	IV
5.	Analyze the importance of electronic spectroscopy and the energy transfer processes	K4	IV
6.	Examine the structure of molecules using the principles of NMR & NQR spectroscopy	K4	V

2A. Syllabus

UNIT-I GROUP THEORY

1.1 Group theory -symmetry of elements and symmetry of operations, point groups of molecules, properties of a group and sub-group, isomorphism, cyclic, abelian, class- similarity transformation and conjugate, matrix representation – product of symmetry operations, group multiplication tables(C_n, C_{nv} and D_{nh} only) - great orthogonality theorem and its consequences, construction of character tables($C_{2V}$and C_{3V}). Direct products – reducible and irreducible representation - Wave function as bases for irreducible representation.

1.2 Crystal point group, crystal symmetry - screw axis and glide plane, space groups, translational elements of symmetry, differences between molecular symmetry and crystal symmetry.

UNIT – II APPLICATIONS OF GROUP THEORY

Group theory and molecular electronic states- Transition moment integral – spectroscopic selection rules to IR, Raman (H_2O, NH_3, trans-N_2F_2) and electronic spectroscopy (HCHO) - projection operators and their use to construct SALC - evaluation of energies and MO's for systems - ethylene, butadiene, benzene and allyl. Hybridization schemes of orbitals – (sp, sp^2 and sp^3)

Xxxx- Revised content

UNIT-III MOLECULAR SPECTROSCOPY-I

3.1 Introductory aspects: electromagnetic radiation -representation of spectra, the line width and intensity of spectral transitions- factors influencing them- Einstein's transition probability and oscillator strength.

3.2 Infrared spectroscopy: Selection rules –harmonic and anharmonic oscillations –rotation and vibrational spectra of polyatomic molecules –CO_2,H_2O-fermi resonance –influence of rotation on the spectra of diatomic molecules –parallel and perpendicular bands.

3.3 Raman spectroscopy: Raman effect –elastic and inelastic scattering –quantum theory – origin of Stokes, Anti-Stokes and Rayleigh lines – selection rules-rotational and vibrational Raman spectra – simple molecules (CO_2, H_2O), mutual exclusion principle – Basics of Laser Raman spectroscopy.

UNIT-IV MOLECULAR SPECTROSCOPY-II

4.1 Electronic spectra: electronic spectra of molecules, Born Oppenheimer approximation, vibrational coarse structure –Frank-Condon principle, dissociation energy, predissociation, rotational fine structure of electronic vibrational transitions – Fortrat diagram- various types of transitions - auxochromes ,chromophores - bathochromic and hypsochromic shift- effect of substituent and polarity of solvent.

4.2 Emission spectroscopy: fate of electronically excited molecules- fluorescence, phosphorescence, emission spectra of molecules.

4.3 Photochemistry: Differences between photochemical and thermal reactions-Quantum yield- Photophysical processes in electronically excited molecules – Jablonski diagram-energy transfer processes – Radiative and Non-Radiative transitions –Fluorescence-relation to structure- Phosphorescence- conditions for Phosphorescence emission (spin-orbit coupling)- Photosensitization – Stern - Volmer equation derivation for quenching of luminescence and quenching of chemical reaction and its applications- Chemiluminescence.

UNIT-V MOLECULAR SPECTROSCOPY-III

5.1 NMR spectroscopy : Energy of interaction and its derivation, Zeeman effect, nuclear spin and applied magnetic field, Effect of 'B' on splitting – Larmor precession and its expression- relaxation processes – PMR – chemical shift - factors affecting chemical shift and coupling constant (J) – spin-spin interaction. ^{13}C NMR spectroscopy – chemical exchange-**Problems.**

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5.2 NQR spectroscopy: characteristics of quadrupolar nucleus- effect of field gradient and magnetic field upon quadrupolar energy levels- NQR transitions – applications of NQR spectroscopy.

5.3 Lasers: Nature of stimulated emission- coherence, monochromaticity, population inversion – cavity and mode characteristics- types of lasers- solid state, gas, chemical and dye lasers.

2B.Topics for Self-Study:

S.No.	Topics	Web Links
1	Problems on Group Theory	https://www.youtube.com/watch?v=UVA42JYBkKw
2	Challenges in application of Raman spectroscopy to biology and materials	https://pubs.rsc.org/en/content/articlepdf/2018/ra/c8ra04491k
3	Sensing genetic disorders with fluorescence	https://chembam.com/online-resources/experiments/sensing-with-fluorescence/
4	Multidimensional NMR Spectroscopy	https://nptel.ac.in/courses/104/108/104108097/
5	The Future of Laser Technology	https://now.northropgrumman.com/the-future-of-laser-technology-hint-its-bright/

2C.Text Books

1. K.V. Raman, "Group Theory and its Application to Chemistry", Tata McGraw-Hill, New Delhi, 2000. **(Unit I, II)**
2. G. Aruldhas, "Molecular Structure and Spectroscopy", Prentice Hall, New Delhi, 2002. **(Unit III, IV, V)**

2D.Reference Books

1. F.A. Cotton, "Chemical Applications to Group Theory", John Wiley and Sons, New York, 2008.
2. Robert. L. Carter, "Molecular symmetry and Group Theory", John Wiley and Sons, New York, 2009.
3. B.E. Douglas and C.A. Hollingsworth, "Symmetry in Bonding and Spectra- an Introduction", Academic Press, 2012.
4. Robert J. Silbey, Robert A. Alberty, "Physical Chemistry", John Wiley and Sons, New York, 2006.
5. G.M. Barrow, "Introduction to Molecular Spectroscopy", McGraw-Hill, New York, 1964.
6. C.N. Banwell and E.M. McCash, "Fundamentals of Molecular Spectroscopy", 4th Edition, Tata McGraw-Hill, New Delhi, 2000.
7. K.V. Raman, R. Gopalan and P.S. Raghavan, "Molecular Spectroscopy", Thomson and Vijay Nicol, Singapore, 2004.
8. I.N.Levine, "Molecular Spectroscopy", John Wiley and Sons, New York, 1974.
9. A.Rahman, "Nuclear Magnetic resonance- Basic Principles", Springer-verlag, New York, 1986.

3.Specific Learning Outcomes (SLO)

Unit	Course Content	Learning Outcomes	Blooms Taxonomic levels of Transaction.
I	**Group Theory**		
1.1	Group theory -symmetry of elements and symmetry of operations, point groups of molecules.	Identify the point group of the given molecule.	K3
		Categorize the molecules based on the point group.	K4
	Properties of a group and sub-group, isomorphism, cyclic, abelian, class-similarity transformation and conjugate, matrix representation.	Classify a group based on the various properties of group.	K4
	Product of symmetry operations, group multiplication tables(C_n, C_{nv} and D_{nh} only)	Summarize the symmetry operations for a point group	K2
		Test for the symmetry operation to form the group from multiplication table	K4
	Great orthogonality theorem and its consequences.	Explain the Orthogonality theorem and its significance	K4
	Construction of character tables ($C_{2V}$and C_{3V}). Direct products – reducible and irreducible representation – Wave function as bases for irreducible representation	Construct the character table for a specific point group.	K3
1.2	Crystal point group, crystal symmetry - screw axis and glide plane, space groups, translational elements of symmetry, differences between molecular symmetry and Crystal symmetry.	Identify the crystallographic space group.	K3
		Classify the crystal symmetry.	K4
II	**Applications of Group Theory**		
2.1	Group theory and molecular electronic states- Transition moment integral	Outline the selection rules for molecular spectroscopy	K2
	spectroscopic selection rules to IR, Raman (H_2O, NH_3, trans-N_2F_2) and electronic spectroscopy (HCHO)	Analyze the molecular symmetry with reference to its spectroscopic outcome.	K4
	projection operators and their use to construct SALC - evaluation of energies and MO's for systems. - ethylene, butadiene, benzene and allyl.	Construct the SALC to calculate Pi bond energy of different systems.	K3

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	Hybridization schemes of orbitals – (sp, sp^2 and sp^3)	Evaluate the hybridized orbital involved in a given molecule by symmetry operation	K5
III	**Molecular Spectroscopy-I**		
3.1	Introductory aspects: electromagnetic radiation -representation of spectra, the line width and intensity of spectral transitions	Outline the introductory aspect of spectroscopy.	K2
		Examine the factors affecting the width and intensity of spectral lines	K4
	Factors influencing them- Einstein's transition probability and oscillator strength.	Explain transition probability and oscillator strength.	K3
		Evaluate oscillator strength.	K4
3.2	Infrared spectroscopy: Selection rules –harmonic and anharmonic oscillations	Show the selection rules for harmonic and anharmonic oscillators.	K2
		Evaluate the anhormonicity value of molecule	K5
	Rotation and vibrational spectra of polyatomic molecules –CO_2, H_2O- fermi resonance	Identify vibrational and rotational frequency of poly atomic molecules.	K3
	Influence of rotation on the spectra of diatomic molecules –parallel and perpendicular bands.	Make use of rotational energy in the vibration level to understand the parallel and perpendicular bands.	K3
3.4	Raman spectroscopy: Raman effect – elastic and inelastic scattering – quantum theory – origin of Stokes, Anti-Stokes and Rayleigh lines	Summarize the basics of Raman scattering.	K2
		Identify the factors affecting scattering	K3
	Selection rules-rotational and vibrational Raman spectra – simple molecules (CO_2, H_2O), mutual exclusion principle – Basics of Laser Raman spectroscopy.	Explain the selection rules for active molecules in Raman spectra.	K3
		Summarize the theory of mutual exclusion principle	K2
		Predict the structure of molecule based on Raman spectra	K5
IV	**Molecular Spectroscopy-II**		

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4.1	Electronic spectra: electronic spectra of molecules, Born Oppenheimer approximation, vibrational coarse structure –Frank-Condon principle, dissociation energy, predissociation.	Explain the basics of electronic spectrum and Frank- Condon principle.	K3
		Summarize the factors influencing predissociation of molecule.	K2
		Calculate dissociation energy of molecule.	K4
	Rotational fine structure of electronic vibrational transitions – Fortrait diagram	Make use of Fortrait diagram	K3
		Predict the effect of rotation on vibrational transition.	K3
	Various types of transitions - auxochromes, chromophores - bathochromic and hypsochromicshift- effect of substituent and polarity of solvent.	Outline the various types of shifts in electronic transition.	K2
		Analyze the effect of substituent on absorption	K3
4.2	Emission spectroscopy: fate of electronically excited molecules- fluorescence, phosphorescence, emission spectra of molecules.	Explain the basics of emission spectroscopy.	K4
		Summarize the energy transfer processes occurring in emission spectra.	K2
V	**Molecular Spectroscopy-III**		
5.1	NMR spectroscopy : Energy of interaction and its derivation, Zeeman effect, nuclear spin and applied magnetic field, Effect of ‘B’ on splitting – Larmor precession and its expression.	Explain the basics of nuclear magnetic resonance spectroscopy.	K2
		Calculate the energy of interaction and processional frequency.	K4
	Relaxation processes – PMR – chemical shift - factors affecting chemical shift and coupling constant (J) –spin-spin interaction. ^{13}C NMR spectroscopy – chemical exchange- Problems**.**	Examine the factors affecting chemical shift and coupling constant	K4
5.2	NQR spectroscopy: characteristics of quadrupolar nucleus- effect of field	Apply NQR principle and spectroscopy.	K3

	gradient and magnetic field upon quadrupolar energy levels- NQR transitions – applications of NQR spectroscopy.		
5.3	Lasers: Nature of stimulated emission- coherence, monochromaticity, population inversion .	Explain the basics of LASER radiation.	K3
		Outline the factors affecting the LASER	K2
	Cavity and mode characteristics- types of lasers- solid state, gas, chemical and dye lasers.	Explain the different types of LASER.	K3
		Construct the LASER sources.	K3

4.Mapping Scheme for the PO, PSOs and COs

L-Low M-Moderate H- High

Course Title: GROUP THEORY & SPECTROSCOPY

Course Code : P19CH409

Mapping	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PSO1	PSO2	PSO3	PSO4
CO1	L	M	H	H	--		--	M	L	M	--	L	M
CO2	M	H		M	--	M	--	--	--	H	--	M	H
CO3	L	M	M	H	M		--	--	L	M	--	L	--
CO4		L	M	M	H		--	L	--	L	H	--	L
CO5		L	M	M	H	M	M	--		L	H	--	--
CO6	M	H		M	--		--	--	--	H	--	M	--

5.Course Assessment Methods

Direct

1. Continuous Assessment Test (Model Exams) I,II
2. Open book test; Cooperative learning report, Assignment; Journal paper review, Group Presentation, Project report, Poster preparation, Proto-type or Product Demonstration etc. (as applicable)
3. End Semester Practical Examination

Indirect

1. Course-end survey

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Xxxx- Revised content

ELECTIVE COURSE: III - APPLICATIONS OF DRUG DESIGN & DISCOVERY

SEMESTER : IV **CODE : P19CH4:3**
CREDITS : 4 **TOTAL HOURS : 75**
Hours/Week:5

1.Course Outcomes

After the successful completion of this course the students will be able to

S.No.	Course Outcomes	Level	Unit
1	Summarize the pharmacokinetics and pharmacodynamics of processes from Drug to Hit	K2	I
2	Evaluate the different modes of drug - receptor interactions	K5	II
3	Propose a Retro-synthetic strategy for the drug molecule	K6	III
4	Employ the principals involved in simple QM & MM Calculations and QSAR procedures for a given drug molecule (K3)	K3	IV
5	Explain the Steps involved in a docking Scheme	K4	V
6	Create and Interconvert Molecular Representations in different electronic formats for further computation and Topological Analysis	K6	V

2A. Syllabus

UNIT- I DRUG DESIGN AND DISCOVERY 15 hours
Historical background- -drug targets: lipids, carbohydrates, proteins ,enzymes, and nucleic acids as drug targets and receptors. Receptor Pharmocology –Agonists and Antagonists(partial and full)- Allosteric Modulators – Pharmacokinetics and pharmacodynamics: administration, absorption, distribution, metabolism, elimination of drugs-bioavailability of drugs-side effects- Case study : serotonin and dopamine receptors and transferring drugs.

UNIT -II DRUG IDENTIFICATION AND VALIDATION 15 hours
Steps in drug discovery – Lead identification- Hits- Drug validation-Natural products as drugs – molecular recognition in drug design – thermodynamic considerations – physical basis and inter molecular interactions between drugs and targets like electrostatic interactions – ionic bonds- hydrogen bonds – Inductive interactions – dispersive forces. Stereochemistry in drug designing – stereospecificity of drug targets – Eudesmic ratio – Examples of Eutomers and Distomers

UNIT - III RETROSYNTHETIC STRATEGIES FOR DRUG SYNTHESIS 15 hours
Introduction to retrosynthetic analysis and disconnection approach – synthons acceptor and donor – synthetic equivalents- umpolungs – planning a synthesis – relay and convergent routes- Guidelines for disconnection – one group C-X and C-C disconnections – Chemoselectivity. Two group C-C disconnections in dicarbonyls – Case Study : Synthesis of Amelfolide.

UNIT- IV COMPUTER AIDED DRUG DESIGN 15 hours

Molecular modeling in drug design – Energy Minimization methods – both Molecular Mechanics and Quantum mechanical Methods –Energy minimization –Conformational analysis –Structure based and Ligand based Drug design –QSAR – parameters –Quantitative models of QSAR – Hansch methods – free Wilson model -3D pharmacophore modeling – Docking – Introduction-Preparation of protein and ligands-Types of docking- rigid and flexible methods of docking -Online docking tools- Post docking analysis.

UNIT -V CHEM INFORMATICS 15 hours

Introduction- Molecular representation and Topological indices -2D & 3D, SMILES-ROSDAL-MDL number, Z-Matrix and Cartesian coordinates-Types of database-Online Cheminformatics database-Chemspider-MOLBASE-ADMET property calculator, DruLiTo, Episuite and molinspiration.

2B.Topics for Self-Study:

S.No.	Topics	Web Links
1	Target based Drug Design – video Lesson	https://www.youtube.com/watch?v=Ir2qIuFMRkE
2	Computer Aided Drug Design Some case studies	https://www.researchgate.net/publication/268924374_Success_Limitation_and_Future_of_Computer_Aided_Drug_Designing
3	AutoDock Exercises	http://autodock.scripps.edu/faqs-help/tutorial
4	Drug Likeliness Tools for practice	http://www.niper.gov.in/pi_dev_tools/DruLiToWeb/DruLiTo_index.html

2C.Text Books

1. Andrew R. Leach, Valerie J Gillet, An Introduction to Cheminformatics, Revised Edition, Springer, Netherland, 2007. **(Unit I, II, IV, V)**

2.Stuart Warren “Organic Synthesis The Disconnection Approach” Wiley; 2nd Edition, 2008 **(Unit III)**

2D.Reference Books

1. Larsen et al,Text book of Drug Design and Discovery,4th Edition, London and Newyork , Taylor and Francis, 2004.
2. Graham L. Patrick, An Introduction to Medicinal Chemistry, 4th Edition, Oxford University Press, 2009.
3. Johann Gasteiger, Thomas Engel, Cheminformatics : A Textbook,Wiley VCH, Weinheim, 2003.

2E.Web links:

To download protein Structures and small molecules : https://www.rcsb.org/
Online Platform for Molecular Description : http://www.scbdd.com/chemdes/

Xxxx- Revised content

3.Specific Learning Outcomes (SLO)

Unit/Section	**Course Content**	**Learning Outcomes**	**Blooms Taxonomic levels of Transaction**
I	**Drug Design And Discovery**		
	Historical background	Recall the various methods & stages of drug design adopted from time to time.	K1
	Drug targets: lipids, carbohydrates, proteins, enzymes, and nucleic acids as drug targets and receptors.	Classify the Targets and receptors based on their chemical and biological	K2
	Receptors Pharmocology – Agonists and Antagonists (partial and full)- Allosteric Modulators	Relate receptors based on types of interactions	K3
		Correlate the activity of different possible drug molecules	K4
	Pharmacokinetics and pharmacodynamics: administration, absorption, distribution, metabolism, elimination of drugs	Estimate the fate of a drug candidate in human body.	K5
	bioavailability of drugs-side effects-	List out rules that connect Properties of candidates to their bioavailability	K2
	Case study: serotonin and dopamine receptors and transferring drugs.	Recollect the principles involved in the design of a suitable drug using transferring receptors	K2
II	**Drug Identification And Validation**		

Xxxx- Revised content

	Steps in drug discovery – Lead identification- Hits- Drug validation	Construct a step wise plan for the design of a known drug	K3

Xxxx- Revised content

	Natural products as drugs	List out the various types of natural sources for drug design	K2
	Molecular recognition in drug design – thermodynamic considerations –	Summarize the role of thermodynamic parameters in the drug target interactions.	K5
	Physical basis and inter molecular interactions between drugs and targets like electrostatic interactions – ionic bonds- hydrogen bonds- Inductive interactions – dispersive forces	Identify the role played by different types of Molecular interactions between drugs & Targets.	K3
	Stereochemistry in drug designing – Stereospecificity of drug targets – Eudesmic ratio – Examples of Eutomers and Distomers	Apply the Eudesmic ratios in appropriate cases of drug design.	K3
III	**Retrosynthetic Strategies For Drug Synthesis**		
	Introduction to retrosynthetic analysis and disconnection approach	Differentiate the retro-synthetic Scheme from a conventional Synthetic Scheme	K4
	Synthons acceptor and donor – synthetic equivalents- umpolungs	Create a Synthon and Synthetic Equivalents for a Targeted Molecule.	K6
	Planning a synthesis – relay and convergent routes-	Compute the percentage yield in different routes of a synthesis. Choose the appropriate route while planning a synthesis	K6
	Guidelines for disconnection – one group C-X and C-C disconnections	Create a synthetic strategy through one group disconnections.	K6

	Chemoselectivity	Evaluate possible routes of synthesis based on selectivity Principles.	K5
	Two group C-C disconnections in dicarbonyls –	Create a synthetic strategy through two group disconnections.	K6
	Case Study : Synthesis of Amelfolide.	Recollect the application of the disconnection approach in synthesis of Amelfolide.	K2
IV	**Computer Aided Drug Design**		
	Molecular modeling in drug design – Energy Minimization methods – both Molecular Mechanics and Quantum mechanical Methods	Apply the basics theoretical background of Molecular Modelling Methods to simple molecular calculations.	K3
	Energy minimization – Conformational analysis	Compare the methods used in different Programs to identify conformers *insilico*	K2
	Structure based and Ligand based Drug design –QSAR – parameters –	Utilise Physical & Chemical Parameters to find out Structure – Activity Relationships	K3
	Quantitative models of QSAR – Hansch methods – free Wilson model -3D pharmacophore modeling	Illustrate the Qualitative models for relevant Drug candidates.	K2
	– Docking – Introduction-Preparation of protein and ligands-Types of docking- rigid and flexible methods of docking	Analyse the steps involved in the docking scheme.	K4
	-Online docking tools- Post docking analysis.	Utilize the free docking tools – Autodock and Hex.	K3
V	**Chem Informatics**		

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	Introduction to Cheminformatics	Describe the features of cheminformatics.	K2
	Molecular representation and Topological indices -2D & 3D, SMILES-ROSDAL-MDL number, Z-Matrix and Cartesian coordinates-	Construct 2D & 3D representations of molecules using Software Tools or Online Programs	K6
	Types of database-Online Cheminformatics database-Chemspider-MOLBASE-	Analyse relevant information from databases useful for Drug Design.	K4
	ADMET property calculator, DruLiTo, Episuite and molinspiration.	Correlate bio-activity of candidates reported in literature to ADMET properties using the different Soft ware to	K4

4. Mapping Scheme for the PO, PSOs and COs

L-Low M-Moderate H- High

Course Title: APPLICATIONS OF DRUG DESIGN & DISCOVERY
Course Code : P19CH4:3

Mapping	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PSO1	PSO2	PSO3	PSO4
CO1	H	-	M	H	L	-	-	-	-	H	M	-	-
CO2	H	M	M	H	L	-	-	-	-	H	L	L	-
CO3	H	H	-	M	L	-	L	L	L	H	H	-	H
CO4	M	H	L	H	M	M	L	-	-	M	-	M	M
CO5	M	M	M	H	M	H	M	L	L	M	M	L	L
CO6	M	M	L	L	H	H	M	-	L	H	M	L	M

5.Course Assessment Methods

DIRECT:

1. Continuous Assessment Test: T1, T2 (Theory & Practical Components): Closed Book
2. Seminar
3. Cooperative Learning Report, Assignment, Group Presentation, Group Discussion, project Report, Field Visit Report, Poster Presentation, Seminar, Quiz (written).
4. Pre-Semester & End Semester Theory Examination

INDIRECT:

1. Course end survey (Feedback)

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ELECTIVE IV: SELECTED TOPICS IN CHEMISTRY

SEMESTER : IV **CODE : P19CH4:4**
CREDITS : 2 **TOTAL HOURS : 75**
Hours/Week :5

1.Course Outcomes:

At the end of this course, the students will be able to:

S.No.	Course Outcomes	Level	Unit
1.	Categorize nanomaterials based on structure and properties	K4	I
2.	Apply nanomaterials in the field of sensors and energy storage devices	K3	II
3.	Summarize the principles and applications of Radiation chemistry in different fields	K4	III
4.	Explain the principle of molecular recognition and supramolecular interactions	K4	IV
5.	Explain the applications of supramolecules in drug delivery systems and electronic devices	K3	IV
6.	Apply the principles of Green Chemistry in chemical processes	K3	V

2A. Syllabus

UNIT – I NANO MATERIALS 15 Hours

Definition, Classification, size dependent, optical and electronic properties of Nanomaterials, Dandling bonds- 1D and 2D Nano structures, CNT and Fullerenes-Quantum dots-Wet methods of synthesis.

UNIT –II APPLICATIONS OF NANOMATERIALS 15 Hours

Application of Nano materials in medicine, drug delivery, agriculture, communication, defence sector, Solar cells, Sensors- Chemical Sensors and Biosensors, super capacitors, pollution treatment.

UNIT –III RADIATION CHEMISTRY 15 Hours

Measurement of dose. Dosimetric terms and units (Roentgen, REM, Rad, Gray, Sievert), inter conversions, calculation of absorbed dose-various types of dosimeters, chemical dosimeters (Fricke, Ceric sulphate and FBX)- Radiolysis of water & hydrated electron. Principle and set up of Radioimmunoassay (RIA) & Immuno-radiometric assay (IRMA)

UNIT –IV SUPRAMOLECULAR CHEMISTRY 15 Hours

Introduction, types of supramolecular interactions, lock and key principle, molecular recognition of different types of guest-host systems, Classification of receptors-cooperative and binding in host-guest systems, molecular hosts-calixarenes, cyclodextrins, cucurbiturils. Dendrimers-Properties and applications, Supramolecular devices- Photonics, logic gates and switching devices.

UNIT –V GREEN CHEMISTRY 15 Hours

Introduction, Anastas twelve principles, Concept of atom economy, some important techniques and directions in practicing green chemistry, use of green solvents- TiO_2 as green photo catalyst, green polymer-chitin, real world examples of green processes.

2B.Topics for Self – Study

S.No.	Topics	Web Links
1	Benefits and Applications of Nanotechnology	https://www.nano.gov/you/nanotechnology-benefits
2	A Review on Chemical and Physical Synthesis Methods of Nanomaterials	https://www.ijraset.com/fileserve.php?FID=13212
3	The Medical, Agricultural, and Industrial Applications of Nuclear Technology	https://www.laradioactivite.com/site/pages/RadioPDF/Waltar.pdf
4	Supramolecular Chemistry-Concepts and Applications	https://www.ijsr.net/archive/v4i4/29031502.pdf
5	Industrial applications of green chemistry: Status, Challenges and Prospects	https://link.springer.com/article/10.1007/s42452-020-2019-6
6	Applications of green chemistry in pharmaceutical chemistry and day today life	https://www.researchgate.net/publication/320033907

2C.Text Books

1. V.K. Ahluwalia, “Methods and Reagents of Green Chemistry: An Introduction by Green Chemistry”, Alpha Science International, 2013. **(Unit-V)**

2. Asim K. Das & Mahua Das, “An Introduction to Supramolercular Chemistry”, CBS Publishers & Distributors PVT ltd., 2005. **(Unit-IV)**

3. Jean- Marie Lehn, “Supramolecular Chemistry Concepts & Perspectives”, Wiley –VCH, 2014. **(Unit-IV)**

4. A. Mozumder, “Fundamentals of Radiation Chemistry” , Academic Press, 1999. **(Unit-II)**

5. F.W. Billmayer. “Textbook of Polymer Science”, Wiley New York, 1991. **(Unit-III)**

6. Shubra Singh M.S. Ramachandra Rao, “Nanoscience and Nanotechnology: Fundamentals of Frontiers”, 2013, Wiley Edition, New Delhi. **(Unit-I)**

2D.Reference Books

1. P. T. Anastas and J.C Warner, “Green Chemistry theory and Practice”, Oxford University press,
Oxford, 1988.

2. T. Pradeep, Nano The Essentials, McGraw Hill-Professional, 2008

3. Specific Learning Outcomes (SLO)

Unit	**Course content**	**Learning Outcomes**	**Blooms Taxonomic levels of Transactions**
	Unit-I : Nano Materials		
1	Nano Materials –Definition	Recall the types & properties of nanomaterials	K2
2	Nano Materials – Classification and Size dependent	Categorize the size of the nano materials with their specific properties	K4
3	Optical and electronic properties of nano materials	Apply the properties of nanomaterials to construct suitable devices	K3
		Identify nanomaterials for suitable applications in opto-electronics	K3
4	Dandling bonds – 1D and 2D Nanostructures	Explain the structure of 1D & 2D nanostructures	K2
5	CNT and Fullurenes	Construct carbon nanotubes for drug delivery systems	K3
6	Quantum dots : Wet methods of synthesis	Explain the wet synthetic methods for quantum dots	K2
	Unit – II: Applications of Nano Materials		

7	Applications of Nano materials in: Medicine, drug delivery, agriculture, defence sector and communication	Apply the application of nanomaterials with specific properties in pharmaceutical, agricultural industrial and communication sectors.	K3
8	Solar cells	Develop the nanomaterials for solar cells	K3
9	Sensors – Chemical Sensors and Biosensors	Develop the nanomaterials suitable for chemical sensors & biosensors	K3
10	Super capacitors	Construct the energy storage devices	K3
11	Pollution treatment	Apply the nanomaterials in pollution control & treatment	K3
	Unit-III: Radiation Chemistry		
12	Measurement of dose – Dosimetric terms and units (Roentgen, REM, Rad, Gray, Sievert), interconversions	Classify the different terms used in radiation chemistry and the various units for radiation dosage	K2
13	Calculation of absorbed dose	Apply the principle of dosimeters to calculate the absorbed dose	K3
14	Various types of dosimeters, chemical dosimeters (Fricke, Ceric sulphate and FBX)	Explain the different types of dosimeters and uses	K2
15	Radiolysis of water & hydrated electron.	Explain the mechanism of radiolysis of water and hydrated electron	K2
16	Principle and set up of Radioimmunoassay (RIA) & Immuno-radiometric assay (IRMA)	Examine the principle of RIA & IRMA for detecting the antigen-antibody concentrations	K4
	Unit – IV : Supramolecular Chemistry		
17	Supramolecular chemistry - Introduction	Explain the importance of supramolecular chemistry	K2
18	Supramolecular chemistry – types of supramolecular interactions	Explain the different types of supramolecular interactions in various molecules	K2

19	Lock and key principle	Illustrate the lock & key mechanism of supramolecules	K2
20	Molecular recognition of different types of guest-host systems	Explain the principle of molecular recognition of guest-host systems	K4
21	Classification of receptors-cooperative and binding in host-guest systems, molecular hosts-calixarenes, cyclodextrins, cucurbiturils.	Choose the different types of molecular receptors for host-guest systems	K3
22	Dendrimers-Properties and applications	Develop the properties of dendrimers suitable for drug delivery stystems	K3
23	Supramolecular devices-Photonics, logic gates and switching devices.	Construct various electronic devices using supramolecules	K3
	Unit-V : Green Chemistry		
24	Green Chemistry - Introduction	Outline the concepts of green chemistry	K2
25	Twelve principles of Green Chemistry	Recall the principles of green chemistry	K2
26	Concept of atom economy	Explain the concept of atom economy of a reaction	K2
27	Some important techniques and directions in practicing green chemistry	Identify the techniques and directions of green chemistry	K3
28	Use of green solvents- TiO_2 as green photo catalyst, green polymer-chitin, real world examples of green processes.	Classify the greener solvents for greener processes	K3

4. Mapping Scheme for the POs, PSOs and Cos for the Course P19CH4:4

L-Low **M-Moderate** **H- High**

Course Title: SELECTED TOPICS IN CHEMISTRY
Course Code: P19CH4:4

Mapping	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PSO1	PSO2	PSO3	PSO4
CO1	H	H	M	M	L	-	H	M	L	M	M	M	M
CO2	H	M	M	M	L	-	H	M	L	M	H	M	M
CO3	M	H	H	M	M	L	H	L	L	M	H	M	M
CO4	M	M	M	M	H	M	M	L	L	L	L	L	L
CO5	M	M	M	L	L	L	M	L	L	M	L	L	L
CO6	H	M	M	M	L	M	H	H	L	M	M	L	M

5. Course Assessment Methods

Direct

1. Continuous Assessment Test (Model Exams) I,II
2. Open book test; Cooperative learning report, Assignment; Journal paper review, Group Presentation, Project report, Poster preparation, Proto-type or Product Demonstration etc. (as applicable)
3. End Semester Practical Examination

Indirect

1. Course-end survey

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Xxxx- Revised content

Elective: V **COMPUTER AIDED MOLECULAR CALCULATIONS**

(PRACTICAL)

Semester: IV **Code: P19CH4:P**
Credits: 2 **Total Hrs :45**

1. Course Outcomes:

At the end of this course, the students will be able to

S.No.	Course Outcomes	Level
1	Construct the chemical structure of molecules using computational tools (K6)	K6
2	Analyze chemical structures using software such as Mercury and JMOL (K4)	K4
3	Interpret the properties of drugs using QSAR study, PDB search, and Regression analysis (K5)	K5
4	Determine different chemical quantities (UV spectra, Adsorption and Toxicity value) using computational software such as DruLiTo, Chemdraw and Argus Lab (K5)	K5
5	Predict the structure and properties of molecules using appropriate computational tools (K5)	K5
6	Inspect the binding efficiency of Pro-drug molecules using docking studies (K4)	K4

2A. Syllabus

EXPERIMENTS:

1. Calculation of ADMET properties of some drugs using DruLiTo (Drug likeliness toxicity)
2. Calculation of the topological and molecular parameters from chemdraw and Chem-3D.
3. Use mathematica and online equation editors to type the given derivation (At least two pages)
4. Retrieving chemical and biological information from online data bases (Swiss prot, NCI, PDB, CCDC).
5. Use of online compound collection data bases (zinc.docking.org, molinspiration)
6. Analyse the hydrogen bonding interaction in the given host guest molecules using HBAT.
7. Regression analysis of the given set of data (MS-Excel)
8. Docking: Small molecule docking using Chemdraw.
9. QSAR a) Calculation of Clog P values
   b) Effect of functional group on activity

c) Drawing QSAR plot based on the QSAR results.

10. Molecular visualization and interconversion using Hg-Mercury, JMOL, chemissian,
11. Prediction of UV-Spectra of the given molecules using Argus Lab.

2B.Text Books:

1. Anand Solomon “Molecular Modeling and Drug Design” MJP Publishers, Chennai, 2008.
2. K.V. Raman “Computers in Chemistry” Tata McGraw Hill, New Delhi, 1993.

2C.Reference Books:

1. Kishore Arora “Computer Applications in Chemistry”, Anmol Publications, New Delhi, 2004.
2. Andrew R. Leach, “Molecular Modeling Principles & Applications”, Prentice Hall, 2nd Edition, 2008.

3.Specific Learning Outcomes (SLO)

S.No	**Course Content**	**Learning Outcomes**	**Blooms Taxonomic levels of Transaction**
1.	Calculation of ADMET properties of some drugs using DruLiTo (Drug likeliness toxicity)	Evaluate the nature of drug using ADMET properties	K5
2.	Calculation of the topological and molecular parameters from Chemdraw and Chem-3D	Predict the molecular topology to understand their reactivity	K6
3.	Use mathematical and online equation editors to type the given derivation (At least two pages)	Utilize online tools for writing equations and fitting into the document	K3
4.	Retrieving chemical and biological information from online data bases (Swiss prot, NCI, PDB, CCDC)	Examine the protein functions by the details obtained from the database	K4
		Deduce the details for molecular docking studies	K4
5.	Use of online compound collection data bases (zinc.docking.org, molinspiration)	Choose the suitable drug from the online data base	K3
6.	Analyse the hydrogen bonding interaction in the given host guest molecules using HBAT	Analyze the stability and structural features of hydrogen bonded host-guest molecules	K4

7.	Regression analysis of the given set of data (MS-Excel)	Apply regression analysis and interpret the given data	K3
8.	Docking: Small molecule docking using Chemdraw	Infer docking studies of simple molecules	K4
9.	QSAR a) Calculation of Clog P values b) Effect of functional group on activity c) Drawing QSAR plot based on the QSAR results	Interpret the property of drugs using structure activity relationship	K5
10.	Molecular visualization and interconversion using Hg-Mercury, JMOL, Chemissian.	Analyze the structure of molecules with the software	K4
11.	Prediction of UV-Spectra of the given molecules using Argus Lab.	Develop the UV-spectra for a given molecule	K3

3.AText Books:

1. Anand Solomon “Molecular Modeling and Drug Design” MJP Publishers, Chennai, 2008.
2. K.V. Raman “Computers in Chemistry” Tata McGraw Hill, New Delhi, 1993.

3B.Recommended Reference Books:

1. Kishore Arora “Computer Applications in Chemistry”, Anmol Publications, New Delhi, 2004.
2. Andrew R. Leach, “Molecular Modeling Principles & Applications”, Prentice Hall,2nd Edition, 2008.
3. F. Jensen, Introduction to computational chemistry, Wiley, New York, 1999.

Mapping Scheme for the POs, PSOs and COs

H - High; M - Moderate; L - Low

Course Title: COMPUTER AIDED MOLECULAR CALCULATIONS
Course Code: P19CH4:P

Mapping	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PSO1	PSO2	PSO3	PSO4
CO1	H	H	M	L	L	H	-	-	-	M	-	-	H
CO2	-	-	L	H	M	-	-	-	-	L	-	-	H
CO3	-	-	L	M	M	H	-	-	-	-	-	M	M
CO4	-	M	M	H	M	H	-	-	-	L	-	-	M
CO5	-	H	L	H	M	H	-	-	-	-	-	H	L
CO6	M	-	-	M	L	H	-	-	-	M		L	M

Xxxx- Revised content

Core Project **CORE PROJECT**

(Theory cum Project)

Semester : IV **Code: P19CH4PJ**
Credits: 4 **Total Hrs : 75**
Hours/week:5

1.Course Outcomes:
At the end of this project, the students will be able to:

S.No.	Course Outcomes	Level
1	Choose an appropriate problem and suitable methodology with respect to the challenges in the field (K5)	K6
2	Survey literature sources for adapting alternate or new methodologies (K4)	K4
3	Compile project findings for presenting the solution to broader audience (K6)	K5
4	Practice ethical and professional values (K3)	K5
5	Justify the findings with relevant scientific evidences (K6)	K5
6	Propose new, sustainable and innovative solutions for real time applications (K6)	K4

2. Syllabus-Nil

3.Specific Learning Outcomes:

Course Content	Learning Outcomes	Blooms Taxonomic Levels of Transaction
Choosing a suitable area of research	Discover a suitable topic relevant to reallife challenges	K2
	Predict open ended Problems	K3
	Develop analytical thinking	K3
	Apply various tools to cite Literature	K3
Objectives and Methodology	Devise the methodology	K4
	Plan for the execution of the project work	K4
	Sketch the work plan	K3
Analysis of Result	Solve the problem through various techniquesand methodologies	K6
Discussion based on data analyzed	Compile and interpret project findings	K6
Report Preparation	Justify results in logical and scientific way	K6

Xxxx- Revised content

	Summarize the findings	K5
Viva-Voce	Defend his findings	K5
	Justify the conclusion	K6
Communicating to Journal	Develop critical thinking	K6
	Plan for collaborations	K4
	Prepare research article	K6

4.Mapping Scheme for the PO, PSOs and Cos

L-Low M-Moderate H- High

Course Title: CORE PROJECT **Course Code: P19CH4PJ**													
Mapping	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PSO1**	**PSO2**	**PSO3**	**PSO4**
CO1	H	H	-	M	H	M	M	M	-	H	H	L	-
CO2	H	M	M	H	H	H	M	-	-	H	H	-	M
CO3	H	H	H	H	H	H	-	M	H	H	H	L	H
CO4	-	-	H	L	L	H	-	H	H	H	M	H	-
CO5	H	H	H	H	H	M	M	M	M	H	H	M	H
CO6	H	M	H	M	M	H	H	H	-	H	H	H	H

5.COURSE ASSESSMENT METHODS

Direct
1. Reviews -1 & 3 2. Viva -Voce (Internal) 3. Viva -Voce (External) 4. Project Report