

M.Sc. Chemistry

SEM	Course Code	Course	Course Title	Ins. Hrs / Week	Credit	Exam Hrs	Marks		Total
							CIA	ESE	
I	20PCH1CC1	Core – I	Ionic, Coordinate Solids, Metallurgy and Nuclear reactions	6	5	3	25	75	100
	20PCH1CC2	Core – II	Organic Reaction Mechanisms, Reagents and Natural Products	6	5	3	25	75	100
	20PCH1CC3	Core – III	Inorganic Estimation and Complex Preparations - Practical	6	4	3	25	75	100
	20PCH1CC4	Core – IV	Organic Preparations and Estimation - Practical	6	4	3	25	75	100
	20PCH1DE1	DSE –I#		6	4	3	25	75	100
	TOTAL				30	22			
II	20PCH2CC5	Core – V	Organic reactions, Stereochemistry and Natural Products	6	5	3	25	75	100
	20PCH2CC6	Core – VI	Theory and Applications of Group Theory and Spectroscopy	6	5	3	25	75	100
	20PCH2CC7	Core – VII	Inorganic Qualitative Analysis and Colorimetric Estimations - Practical	6	4	3	25	75	100
	20PCH2CC8	Core – VIII	Qualitative Analysis of Organic Mixture Chromatography Techniques Practical	6	4	3	25	75	100
	20PCH2DE2	DSE–II #		6	4	3	25	75	100
	TOTAL				30	22			
III	20PCH3CC9	Core – IX	Solid State, NMR, ESR, Photo Spectroscopy and Bio-Medicinal Chemistry	6	5	3	25	75	100
	20PCH3CC10	Core – X	Organic Spectroscopy and Natural Products	6	5	3	25	75	100
	20PCH3CC11	Core – XI	Chemical Process in Industry	6	4	3	25	75	100
	20PCH3CC12	Core – XII	Physical Practical	6	4	3	25	75	100
	20PCH3DE3	DSE –III#		6	4	3	25	75	100
	20PCH3EC1	Extra Credit Course-I	Online Course (MOOC)	-	5*	3	-	100	100*
	TOTAL				30	22			
IV	20PCH4CC13	Core – XIII	Classical, Statistical Thermodynamics and Surface Phenomena	6	5	3	25	75	100
	20PCH4CC14	Core – XIV	Chemistry of Macromolecules	6	5	3	25	75	100
	20PCH4CC15	Core – XV	Physical Practical	6	5	3	25	75	100
	20PCH3DE4	DSE –IV#		6	4	3	25	75	100
	20PCH4PW	Project		6	4	-	-	100	100
	20PCNOC	Online Course (Compulsory)		-	1	-	-	-	-
	20PCH4EC2	Extra Credit Course – II	Chemistry for Career Examinations	-	5*	3	-	100	100*
	TOTAL				30	24			
GRAND TOTAL						90			2000

*Not considered for grand total and CGPA

#Discipline Specific Electives

Semester	Course Code	Discipline Specific Elective
I	20PCH1DE1A	Quantum Chemistry, Kinetics of Solutions and Electrodes
	20PCH1DE1B	Quantum Chemistry and Spectroscopy
II	20PCH2DE2A	Chemistry of Complexes and Organometallics, IR, Electronic and Mossbauer Spectroscopy
	20PCH2DE2B	Spectroscopy of Inorganic Complexes and Organometallics
III	20PCH3DE3A	Medicinal Chemistry
	20PCH3DE3B	Chemistry of Material Science
IV	20PCH3DE4A	Green and Nano Chemistry
	20PCH3DE4B	Environmental Chemistry and Quality Control

Semester	Code	Course	Title of the Course	Hours	Credits	Max. marks	Internal marks	External marks
I	20PCH1CC1	Core – I	IONIC, COORDINATE SOLIDS, METALLURGY AND NUCLEAR REACTIONS	6	5	100	25	75

Course Outcomes:

1. Examine the crystal type and defects.
2. Solve CFSE for co-ordination compounds.
3. Design various processes in extraction of metals and manufacture of alloys.
4. Apply various concepts of acids and bases to interpret the types of materials.
5. Investigate radioactivity using detectors and analyse various nuclear reactions.

UNIT– I

18 hours

Crystal Structure

- 1.1 Packing of ions in crystals - Radius ratio rules – Calculation of limiting ratios for coordination number 3 to 6. Classification of ionic structures - AX type (ZnS, NaCl, NiAs, CsCl) and AX₂ type (CaF₂, TiO₂, CdI₂) - structures only.
- 1.2 Defects in crystals: #Schottky and Frenkel defects#-stoichiometric and non-stoichiometric - Metal excess defects - F-Centre. Metal deficiency defects – Positive ion deficiency – extra interstitial negative ions. Semiconductor systems isoelectronic with silicon and their applications – as transistors, as photovoltaic cells. Superconductors – high temperature super conductors.
- 1.3 Lattice energy - Born-Lande equation – significance, Kapustinski equation.

UNIT– II

18 hours

Covalent and coordinate bonds

- 2.1 Covalent bond - M.O. theory – Symmetry and overlap – construction of molecular orbitals in homo and hetero nuclear diatomic molecules. Isoelectronic molecules and ions.
- 2.2 Coordinate bonds - Crystal field theory – Splitting of d-orbitals in O_h Symmetry – Strong and weak fields – CFSE – Calculation. Splitting in T_d symmetry and tetragonal symmetry – Jahn-Teller distortion - splitting pattern in square planar. #Factors affecting the magnitude of 10 Dq value# - Nature of the ligands - Spectrochemical series, Jorgensen's relation. π bonding and MO theory - Ligands with filled and empty π orbitals – Nephelauxetic effect.

UNIT – III

18 hours

- 3.1. **Extraction and Uses of Metals:** Metallurgy of Zr, Ge, Th and U – #uses of their important compounds#
- 3.2. **Alloys and Intermetallic Compounds:** Effect of alloying, types of alloys – simple mixtures, solid solutions, substitutional alloys, interstitial alloys, Intermetallic compounds – Hume-Rothery's rules. Ferrous alloys – Definition, properties and uses. Non-ferrous alloys – types, applications.
- 3.3. **Inorganic polymers:** Phosphorous based network polymers – ultraphosphate glasses, borophosphate glasses - Applications. Coordination polymers - natural and synthetic coordination polymers.
- 3.4. **Rings:** Preparation and Structure of Borazines & Phosphazenes – Craigg and Paddock model - Dewar model – Preparation and Structure of sulphur-nitrogen ring system (S₄N₄, N₄S₄F₄)

UNIT-IV**18 hours****Acids & Bases and solvents**

- 4.1. Non-protonic concepts of acid-base reactions – Lux-Flood concept - Usanowich concept. Hard and soft acids and bases (HSAB Principle) – Classification, acid and base strength of hardness and softness – electro negativity of hardness and softness – applications of HSAB, Symbiosis. Differentiating and leveling solvents.
- 4.2. Solvents general behavior, P.T of ionizing solvents, classification- protic and aprotic solvents - liq. NH₃, SO₂, CH₃COOH, BrF₃ and [#]HF[#].

UNIT- V**18 hours****Nuclear Reactions**

- 5.1. Radioactivity - orbital electron capture, nuclear isomerism, internal conversion.
- 5.2. Detection and determination of radioactivity: Nuclear radiation – Scintillation and Cherenkov Counter. Particle accelerators: Linear, Cyclotron, Synchrotron, Betatron and Bevatron - [#]Nuclear reactors[#]
- 5.3. Reactions - Transmutation, stripping and pick-up, spallation, fragmentation and scattering reactions – Sources of neutrons – Neutron activation and isotopic dilution analysis – applications.

..... # - Self Study Portion

Text Books:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1	J. D. Lee	A New Concise Inorganic Chemistry	5 th Edition	Oxford University Press	2011
2	Wahid U. Malik, G. D. Tuli and R. D. Madan	Selected Topic in Inorganic Chemistry	-	S. Chand & Co., New Delhi	2011
3	Gurdeep Raj	Advanced Inorganic Chemistry-Vol.-I	-	Krishna's Educational Publishers	2014
4.	H.J. Arnikar	Essential of Nuclear Chemistry	4 th Edition	New Age International Publishers	2011

Books for Reference:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1.	Cotton and Wilkinson	Advanced Inorganic Chemistry	6 th Edition	John Wiley & Sons, New York	2004
2.	James E. Huheey, Ellen A. Keiter and Richard L. Keiter	Inorganic Chemistry Principles of Structure and Reactivity	4 th Edition	Pearson Education, 11 th Impression	2011
3.	Bodie E. Douglas D. McDaniel and John Alexander	Concepts and Models of Inorganic Chemistry	3 rd Edition	Wiley India Pvt. Ltd., New Delhi	2006
4.	Peter Atkins, Tina Overton, Jonathan Rourke, Mark Weller and Fraser Armstrong	Inorganic Chemistry	4 th Edition	Oxford University Press, New Delhi	2010
5.	Maheswar Sharon and Madhuri Sharon	Nuclear Chemistry		Ane books Pvt. Ltd., New Delhi	2009

Web References:

https://nptel.ac.in/content/syllabus_pdf/104101121.pdf

Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes:

Semester	Code	Title of the Paper					Hours	Credits			
I	20PCH1CC1	IONIC, COORDINATE SOLIDS, METALLURGY AND NUCLEAR REACTIONS					6	5			
Course Outcomes (COs)	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)					
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	
CO1	✓	✓		✓	✓	✓	✓		✓	✓	
CO2	✓	✓		✓	✓	✓	✓	✓	✓	✓	
CO3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
CO4	✓	✓		✓		✓	✓		✓	✓	
CO5	✓	✓	✓	✓		✓	✓		✓	✓	
Number of Matches = 42, Relationship : High											

Prepared by:

1. Dr.K. Loganathan
2. Dr.N. Mujafarkani

Checked by: Dr.A.Jamal Abdul Nasser

Semester	Code	Course	Title of the Course	Hours	Credits	Max. marks	Internal marks	External marks
I	20PCH1CC2	Core – II	ORGANIC REACTION MECHANISMS, REAGENTS AND NATURAL PRODUCTS	6	5	100	25	75

Course Outcome:

1. Apply the IUPAC nomenclature for different types of organic compounds.
2. Formulate the reagents used for the synthesis of novel organic compounds.
3. Analyse the role of substrate, solvent, attacking nucleophile in the nucleophilic and electrophilic substitution reactions.
4. Categorize different types of addition and elimination reactions.
5. Examine the structure of steroids, carotenoids, flavones and their related compounds

UNIT-I

18 hours

Nomenclature and Reaction Mechanism

1.1. Nomenclature of organic compounds: Nomenclature of alicyclic – #monocyclic#, bicyclic and tricyclic. Nomenclature of heterocycles, having not more than two hetero atoms such as oxygen, nitrogen and sulphur, allenes, spirenes and spiro compounds.

1.2. Reaction intermediates: Singlet oxygen, nitrenes and benzyne – generation, stability, structure and reactivity. Non-classical carbo cations definition, generation and stability.

1.3. Methods of determining reaction mechanism:

Energy profile diagrams - Thermodynamic and kinetic control of organic reactions – intermediate versus transition state - isotopic effects – kinetic and non – kinetic methods of determination of reaction mechanisms – product analysis and its importance – cross over experiment – isotopic labelling studies – stereo chemical studies.

1.4. Correlation analysis: Linear free energy relations – Hammett equation – significance of sigma (σ) and rho (ρ) – applications, deviations and limitations – Taft equation and applications.

UNIT-II

18 hours

Reagents in Organic Synthesis

2.1. Reducing Reagents: Reduction of CO to CH₂ in aldehydes and ketones - Wolff-Kishner reduction and Huang-Minlon modification. Metal hydride reduction - NaCNBH₃, Na(OAc)₃BH, Reduction by dissolving metals–sodium-liquid alcohol, sodium-liquid ammonia. Tin-hydrochloric acid, Zinc-hydrochloric acid, zinc-acetic acid, Magnesium-amalgam. Stannous chloride, sodium metabisulphite and Baker's Yeast.

2.2. Oxidizing Reagents: K₂Cr₂O₇/SO₄ (Jones reagent), Selenium dioxide CrO₃-pyridine (Collin's reagent), PCC (Corey's reagent), hypervalent iodine reagents (IBX, Dess-Martin periodinane), DMSO based reagents (Swern oxidation). Oxidation involving C-C bond cleavage using HIO₄, CrO₃ (cycloalkanones). Oxidation of C=C using NaIO₄ and OsO₄, aromatic rings using RuO₄. Oxidation of aldehydes and ketones with H₂O₂ (Dakin reaction), with peracid (Baeyer-Villiger oxidation).

UNIT-III

18hours

Substitution Reactions

3.1. Aliphatic nucleophilic substitution:

[#]SN¹, SN² and SNⁱ mechanisms[#] - Effect of substrate structure, leaving group, attacking nucleophiles and solvent. Neighbouring group participation - Substitution at norbornyl, bridgehead systems, allylic & vinylic carbons and substitution by ambident nucleophiles.

3.2 Aliphatic electrophilic substitution:

SE¹, SE² and SEⁱ mechanism - Reactivity. Effect of substrate, leaving group, attacking electrophiles and solvent. Keto-enol interconversion, Stark-Enamine reaction, halogenation of aldehydes and ketones and decarboxylation of aliphatic acids.

3.3 Aromatic nucleophilic and electrophilic substitutions:

Aromatic nucleophilic substitution - Unimolecular, bimolecular and benzyne mechanisms. Zeigler alkylation, Chichibabin reaction. Arenium ion mechanism. Isolation of arenium ion intermediates, isotope effects.

Aromatic electrophilic substitution - SE^1 mechanism, orientation & reactivity in mono substituted benzene rings, ortho/para ratio, ipso attack, orientation in benzene rings with more than one substituents.

UNIT-IV

18 hours

ADDITION AND ELIMINATION REACTIONS

4.1. Addition Reactions: Addition to carbon-carbon multiple bonds – Electrophilic addition, nucleophilic and free radical additions, orientation and reactivity, Hydroxylation, Hydroboration, Epoxidation, Diels-Alder reaction. Michael addition, Ozonolysis, 1,3 – dipolar addition reaction . Stereochemical studies in addition reactions. Addition to carbonyl and conjugated carbonyl system-Mechanism – Grignard reagents – 1,2 and 1,4-additions (dimethylithiumcuprate), Benzoin, Knoevenagel, Stobbe and Darzen's glycidic ester condensation and Reformatsky reactions.

4.2 Elimination Reaction: α -Elimination, β -elimination, E_1 , E_2 and E_1CB mechanism – stereochemistry of elimination – orientation of the double bond – effect of changes in the substrate, base, leaving group and medium on E_1 , E_2 , E_1CB reactions. Elimination Vs Substitution – pyrolytic cis elimination – Bredt's rule-Hofmann degradation, Cope elimination -Chugaev reaction – dehydration of alcohols – dehydrohalogenation.

UNIT-V

Steroids, Carotenoids and Flavones

18 hours

5.1 Steroids: Classification – Structural elucidation and medicinal values of cholesterol (synthesis not required), oestrone, equilenin and progesterone, stereochemistry of steroids.

5.2 Carotenoids: Classification, structural elucidation of α -carotene, β - carotene and xanthophylls.

5.3 Flavones: Structural elucidation of flavone, flavanol and isoflavone.

TEXT BOOKS:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1.	Raj K. Bansal	Heterocyclic Chemistry	5 th	New Age International Publishers	2014
2.	V.K. Ahulwalia & Rakesh Kumar	Organic Reaction Mechanism	3 rd	Narosa Publishing House	2009
3.	K.S. Mukherjee	Mechanism of Organic Chemistry	2 nd	Arunabha Sen., Books & Allied (P) Ltd.	2010
4.	Francis A. Carey Richard J. Sunberg	Advanced Organic Chemistry	5 th	Springer International Edition	2012
5.	Gurdeep Chatwal	Organic Chemistry of Natural Products	Vol.I & II Revised 5 th Edition	Himalaya Publishing House	2005

Books for Reference:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1	F.A.Carey and R.J.Sund berg	Advanced organic Chemistry	Vol I and II – 3 rd Edition.	Plenum Publications.	1984
2	S.P. Shukla and G.L Trivedi	Modern Organic Chemistry	Millinium Edition	Rajendran Printers Pvt. Ltd., New Delhi	2000
3	O.P. Agarwal	Reactions and Reagent in Organic	5 th Edition	Goel Publishing House ,Meerut.	2005

		Chemistry			
4.	J.N. Gurtu and R.Kapoor	Organic Reactions and Reagents	1 st Edition	Sultan Chand Company Pvt.Ltd.	1988
5.	R.O.C Norman	Principles of Organic Synthesis	2 nd Edition	Chapman and Hall Publications	1986

Web Reference: https://swayam.gov.in/nd2_ugc19_ch01/preview

Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes:

Semester	Code		Title of the Paper			Hours	Credits			
I	20PCH1CC2		ORGANIC REACTION MECHANISMS, REAGENTS AND NATURAL PRODUCTS			6	5			
Course Outcomes (COs)	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓			✓	✓	✓		
CO2	✓	✓	✓	✓		✓	✓	✓	✓	✓
CO3	✓	✓	✓			✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO5	✓	✓	✓		✓	✓	✓	✓	✓	
Number of Matches = 41, Relationship : High										

Prepared by:

1. Dr. J. Sirajudeen
2. Dr. K. Riaz Ahmed

Checked by: Dr. M. Mohamed Sihabudeen

Semester	Code	Course	Title of the Course	Hours	Credits	Max. marks	Internal marks	External marks
I	20PCH1CC3P	Core –III	INORGANIC ESTIMATION AND COMPLEX PREPARATIONS - PRACTICAL	6	4	100	25	75

Course Outcomes:

1. Apply appropriate methods of precipitation to distinguish metal ions.
2. Determine the concentration of analyte by precipitation technique.
3. Estimate the amount of metals present in the mixture.
4. Synthesize the metal complexes.
5. Perform the analysis of ores and industrial materials

Volumetry, Gravimetry / Complexometric and complex preparations:

Estimation of the following elements by volumetric and gravimetric/complexometric methods:

1. Cu (V) Ni (G/C)
2. Cu (V) Zn (G/C)
3. Cu (V) Mg (G/C)
4. Zn (V) Cu (G/C)
5. Fe (V) Zn (G/C)

Note: V - Volumetric
G -Gravimetric
C -Complexometric

Preparations:

1. Tetramminecopper(II)sulphate
2. Potassiumtrioxalatochromate(III)
3. Hexathiourealead(II)nitrate
4. Potassiumtrioxalatoaluminate(III)
5. Trithioureacopper(I)chloride
6. Trithioureacopper(II)sulphate

Scheme of valuation

Procedure writing -10 marks
Viva -10 marks

Results:

1-2% - 60 marks
2-3% - 50 marks
3-4% - 40 marks
>4% - 30 marks

Semester-I

Text Books:

S.No.	Author Name	Book Name	Edition	Publisher detail	Year
1.	Vogel A I	A Text Book of Quantitative Inorganic Analysis	3 rd Edition	Longman Group	1972
2.	Vogel A I	Text Book of Macro and Semimicro Qualitative Inorganic Analysis	5 th Edition	Longman Group	1979

Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes:

Semester	Code	Title of the Paper	Hours	Credits						
I	20PCH1CC3P	INORGANIC ESTIMATION AND COMPLEX PREPARATIONS - PRACTICAL	6	4						
Course Outcomes (COs)	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓		✓		✓	✓	✓		
CO2	✓	✓		✓		✓	✓	✓		
CO3	✓	✓		✓		✓	✓	✓		
CO4	✓	✓		✓		✓	✓			✓
CO5	✓	✓		✓	✓	✓			✓	✓
Number of Matches = 31, Relationship : Moderate										

Prepared by:

1. Dr.M.Syed Ali Padusha
2. Dr. F. M. Mashood Ahamed

Checked by:

Dr. A. Jamal Abdul Nasser

Semester	Code	Course	Title of the Course	Hours	Credits	Max. marks	Internal marks	External marks
I	20PCH1CC4P	Core –IV	ORGANIC PREPARATIONS AND ESTIMATIONS - PRACTICAL	6	4	100	25	75

Course Outcomes:

1. Design a reaction procedure for the synthesis of compounds
2. Prepare the organic compounds and ensure the purity applying the appropriate techniques
3. Perform recrystallisation process for organic compounds
4. Appraise the quantitative method for the essential organic compounds
5. Understand the principle and estimation techniques of organic compounds

Two Stage Preparations:

25 Marks

- Acetylsalicylic acid from methylsalicylate
- 1,3,5 – Tribromobenzene from Aniline
- *p*-Nitroaniline from acetanilide
- *p*-Bromoaniline from acetanilide
- Benzoic acid from benzoin
- Benzaldehyde to chalcone epoxide via chalcone
- Cyclohexanone to caprolactone via cyclohexanone oxime

Quantitative analysis of organic compounds:

50 Marks

- Estimation of Phenol
- Estimation of Aniline
- Estimation of Ethyl methyl ketone
- Estimation of Glucose
- Estimation of Ascorbic acid

Viva-voce

05 Marks

Scheme of valuation

Organic Estimation

Procedure writing - 10 marks

Results:

1-2% - 50 marks
 2-3% - 40 marks
 3-4% - 30 marks
 >4% - 20 marks

Organic Preparation - 25 marks

Text Books:

S.No.	Author Name	Book Name	Edition	Publisher detail	Year
1.	Vogel A I	A Text Book of Practical Organic Analysis	5 th Edition	Longman Group	1989

Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes:

Semester	Code	Title of the Paper					Hours	Credits		
I	20PCH1CC4P	ORGANIC PREPARATIONS AND ESTIMATIONS - PRACTICAL					6	4		
Course Outcomes (COs)	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓				✓	✓	✓		
CO2	✓	✓	✓		✓	✓	✓			✓
CO3	✓		✓	✓		✓	✓	✓		✓
CO4	✓	✓		✓		✓	✓			✓
CO5	✓	✓	✓	✓		✓	✓			✓
Number of Matches = 32, Relationship : Moderate										

Prepared by:

1. Dr. A. Zahir Hussain
2. Dr. A. Asrar Ahamed

Checked by: Dr. M. Mohamed Sihabudeen

Semester	Code	Course	Title of the Course	Hours	Credits	Max. marks	Internal marks	External marks
I	20PCH1DE1A	DSE –I	QUANTUM CHEMISTRY, KINETICS OF SOLUTIONS AND ELECTRODES	6	4	100	25	75

Course outcome:

1. Apply quantum mechanics in solving SWE to single and much particle system.
2. Construct slaters determinant to molecules and to solve it.
3. Evaluate HMO theory to organic molecules.
4. Discuss the kinetics of solution, fast reactions and catalyzed reactions.
5. Compare the different theories of multiple layers and appreciate their significance.

UNIT – I

18hours

Basic concepts of Quantum Mechanics

1.1. Classical mechanics – #General principles, basic assumptions, postulates of classical mechanics, conservation laws, Lagrange’s and Hamilton’s equations of Motion (no derivation)#. Functions – Definition, Implicit and explicit functions, odd and even functions, integrals of odd and even functions, set of functions, Eigen functions and Eigen values, orthogonality, normalization, orthonormal functions.

1.2.Operators - algebra of operators, commutation relations, linear, angular momentum, Laplacian, Hermitian and Hamiltonian operator, Hermitian property of operators.

1.3. Postulates of quantum mechanics – Solving the Schrodinger wave equation (SWE) to simple systems viz., particle in a box – one and three dimensional, Bohr’s Correspondence principle (Problems from functions, operators, 1D and 3D box).

UNIT – II

18 hours

Applications of Quantum Mechanics-I

2.1 Setting and solving Schrödinger wave equation for harmonic oscillator, rigid-rotator, hydrogen and hydrogen like atoms (He^+ and Li^{2+}). Significance of n, l and m. Shapes of atomic orbitals - radial and angular probability distribution functions.

2.2 Approximation methods - linear variation principle, application to hydrogen and helium atoms, perturbation method for non-degenerate systems, application of perturbation theory to helium atom.

UNIT-III

18 hours

Applications of Quantum Mechanics-II

3.1 Two electron systems – symmetric and anti-symmetric wave functions, spin of electrons and Pauli’s principles and Slater determinant, self-consistent field theory - Hartree-Fock Self Consistent field theory, Slater type orbitals – Slater rules, orbital energies.

3.2 Theory of chemical bonding (diatomic molecules) – Born-Oppenheimer approximation, LCAO-MO and VB treatments of the hydrogen molecule, Huckel’s molecular orbital (HMO) theory and its applications to ethylene, allyl radical and butadiene (linear), principle of hybridization – sp, sp^2 and sp^3 .

UNIT-IV

18 hours

Kinetics of Solutions, Catalysis and Fast reactions

4.1 Factors influencing reaction rates in solutions. Application of ARRT to solution kinetics. Effects of solvents - double sphere and single sphere model and effect of ionic strength. Influence of pressure on reaction rates in solution - significance of volume of activation.

4.2. **Homogeneous catalysis:** #Acid-Base catalysis – General and specific Acid-Base catalysis. Acidity function - Hammett-Dearyup acidity function, Bronsted catalytic law#. Enzyme catalysis - Michaelis-Menten law, influence of pH and temperature on enzyme catalysis.

4.3 **Fast reactions:** Study of kinetics by stopped flow technique, relaxation methods - T and P Jump methods,

UNIT- V**18hours****Electro Kinetic Phenomena and Electrode Kinetics**

5.1 #Debye-Huckel-Onsager theory of strong electrolytes, Debye Huckel limiting law[#], activity coefficient at higher concentration - Bjerrum model. Electrical double layer potential – zeta potential, theory of multiple layers at electrode - Helmholtz, Goy-Chapmann, Stern, Devanathan models. Electro kinetic phenomena – electrophoresis, electrosmosis, streaming potential and sedimentation potential. Electro capillary phenomena – Capillary Rise method and Determination of interfacial tension.

5.2. Process at Electrode – Rate of Charge Transfer- Current Density – Butler-Volmer equation – Tafel equation.

5.3. Principles of Electro deposition of Metals. Electro chemical corrosion of Metals - Construction and use of Pourbaix and Evans diagrams. Prevention of Corrosion – Electro Chemical oxidation and Reduction.

#Self study#

Text Books:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1.	A. K. Chandra	Introductory Quantum Chemistry	4 th Edition	Tata – McGraw Hill	2010
2.	R. K. Prasad	Quantum Chemistry- Through Problems and Solutions	2 nd Edition	New Age Publications	1997
3.	J.M. Anderson	Mathematics of Quantum Chemistry	Revised Edition	Dover Publications	2005
4.	John O'M Bockris and A. K.N. Reddy	Modern Electrochemistry	Volume 2	Anne Book India	2008
5	Laidler	Chemical Kinetics	3 rd Edition	Pearson Publisher	2003
6	Kuriacose and Rajaram	Kinetics and Mechanism of Chemical Transformation	2 nd Edition	Mcmillan & Co	2000

Books for Reference:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1.	F. L. Pillar	Elementary Quantum Chemistry	2 nd Edition	Dover Publications, INC. Mineola, New York	2001
2.	I. N. Levine	Quantum Chemistry	7 th edition	Prentice Hall OfInia, Pvt. Ltd,	2016
3.	James House	Fundamentals of Quantum Chemistry	2 nd Edition	Academic Press	2003
4.	D.R. Crow	Principles and Applications of Electrochemistry	4 th edition	Chapman and Hall, London,	2004
5.	P. H. Rieger	Electro Chemistry	2 nd Edition	Springer-Science Business media	1993

Web Reference:Unit-I and II; www.nptel.ac.in/courses/104108057/

Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes:

Semester	Code	Title of the Paper					Hours	Credits				
I	20PCH1DE1A	QUANTUM CHEMISTRY, KINETICS OF SOLUTIONS AND ELECTRODES					6	4				
Course Outcomes (COs)	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)						
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5		
CO1	✓			✓	✓	✓	✓			✓		
CO2	✓	✓		✓	✓	✓	✓			✓		
CO3	✓			✓	✓	✓	✓	✓		✓		
CO4	✓		✓	✓	✓	✓	✓	✓	✓	✓		
CO5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		
Number of Matches = 39, Relationship : Moderate												

Prepared by:

1. Dr. A. JAFAR AHAMED
2. Dr. M. SYED ALI PADUSHA

Checked by: Dr. M. SEENI MUBARAK

Semester	Code	Course	Title of the Course	Hours	Credits	Max. marks	Internal marks	External marks
I	20PCH1DE1B	DSE -I	QUANTUM CHEMISTRY AND SPECTROSCOPY	6	4	100	25	75

Course outcome:

1. Apply quantum mechanics in solving SWE to single and much particle system.
2. Evaluate HMO theory to organic molecules.
3. Differentiate the principles of different spectroscopies.
4. Assess the principles and applications of NMRI, FT-NMR and Solid state NMR.
5. Compare the applications and advantages of conventional NMR and 2D-NMR

UNIT – I

18 hours

Classical Mechanics and Quantum Mechanics

1.1. Classical mechanics – General principles, basic assumptions, postulates of classical mechanics, conservation laws, D'Alembert's principle, Lagrange's and Hamilton's equations of motion (no derivation). Operators- algebra of operators, commutation relations, commutators, linear, angular momentum, Laplacian, Hermitian, Hamiltonian and Ladder operators, eigen values and eigen functions, Hermitian property of operators, #orthogonality and normalization#.

1.2. Postulates of quantum mechanics – discussion of the Schrödinger wave equation to simple systems viz., particle in a box – one and three dimensional, quantum numbers, harmonic oscillator – zero-point energy, Bohr's Correspondence principle, rigid-rotator- rotational and vibrational quantum numbers, Hydrogen and hydrogen like atoms (He⁺ and Li²⁺), #significance of n, l and m, shapes of atomic orbitals – radial and angular probability distribution functions#.

UNIT-II

18 hours

Application of Quantum Mechanics to Multi electronic Systems:

2.1. Approximation methods - linear variation principle, application to hydrogen and helium atoms, perturbation method for non degenerate systems, application of perturbation theory to helium atom.

2.2. Two electron systems – symmetric and antisymmetric wave functions, spin of electrons and Pauli's principles and Slater determinant, self consistent field theory - Hartree's theory, Hartree-Fock-Self-Consistent field theory, #Slater type orbitals – slater rules, orbital energies#.

2.3. Theory of chemical bonding (diatomic molecules)-Born-Oppenheimer approximation, LCAO- MO and VB treatments of the hydrogen molecule, Huckel molecular orbital (HMO) theory and its applications to conjugated systems - ethylene, allyl radical and butadiene(linear) principle of hybridization-sp, sp² and sp³

Self study

UNIT-III

18 hours

3.1.Theory of IR and Raman spectroscopy:

Einstein coefficient of absorption and transition probabilities – basics selection rules – representation of spectra – the width and intensity spectral transitions – oscillator strength. Vibration spectra – selection rules– harmonic and anharmonic oscillators – hot band, overtones – Fermi resonance, combination bands, rotation – vibration spectra of diatomic molecules – transition for the rigid rotor – coupling of rotation and vibration– linear and perpendicular bonds – FT-IR spectroscopy. #PQR – branches#.

3.2.Raman Spectroscopy:

Raman Effect – elastic and inelastic scattering – selection rules – pure rotational and rotational-vibrational Raman spectra – polarization of light and Raman Effect – mutual exclusion principle – #Fermi resonance – laser Raman spectroscopy#.

UNIT-IV

18 hours

4.1. THEORY OF NMR-I

Behavior of a bar magnet in a magnetic field – Magnetization vectors – resonance condition – relaxation process – Bloch equation – chemical shift and its measurement. Scalar Spin-Spin Coupling Mechanism – Nature of the Coupling, Direct Dipolar Coupling – NMR in Solids – magic angle spinning – #nuclear magnetic resonance imaging (NMRI) – principles and applications#.

4.2. FT-NMR – Principle, Measurements of T1 by FTS, Use of T1 for peak assignment.

UNIT – V

18 hours

THEORY OF NMR-II

5.1. Second Order Spectra – Introduction, More Complicated Second Order System , Double Resonance and Spin Tickling Experiments - elementary idea, Spectral Simplification. Evaluation of thermodynamic data with NMR – Rate constants and activation energies from NMR – Determination of reaction orders by NMR #some application of NMR kinetic studies#.

5.2. Two dimensional NMR –Theory of 2D NMR (preliminary)

Text Books:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1.	A. K. Chandra	Introductory Quantum Chemistry	4 th Edition	Tata – McGraw Hill	2010
2.	R. K. Prasad	Quantum Chemistry- Through Problems and Solutions	2 nd Edition	New Age Publications	1997
3.	J. M. Anderson	Mathematics of Quantum Chemistry	Revised Edition	Dover Publications	2005
4.	C. N. Banwell and E. M. Mccash,	Fundamentals of Molecular Spectroscopy	Fourth Edition (Indian Edition)	Tata McGraw-Hill Publishing Company Limited, New Delhi,	2017

Books for Reference:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1.	F. L. Pillar	Elementary Quantum Chemistry	2 nd Edition	Dover Publications, INC. Mineola, New York	2001
2.	I. N. Levine	Quantum Chemistry	7 th edition	Prentice Hall OfInia, Pvt. Ltd,	2016
3.	James House	Fundamentals of Quantum Chemistry	2 nd Edition	Academic Press	2003
4.	G. Aruldas	Molecular structure and spectroscopy	2 nd edition	PHI learning Pvt. Ltd., New Delhi	2016
5.	David. W. Ball	Physical Chemistry	2 nd Edition	Cengage Learning India Pvt. Ltd., New Delhi	2017

Web Reference:

Unit-I; www.nptel.ac.in/courses/104108057/

Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes:

Semester	Code	Title of the Paper					Hours	Credits				
I	20PCH1DE1B	QUANTUM CHEMISTRY AND SPECTROSCOPY					6	4				
Course Outcomes (COs)	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)						
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5		
CO1	✓			✓	✓	✓				✓		
CO2	✓	✓			✓	✓				✓		
CO3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		
CO4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		
CO5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		
Number of Matches = 40, Relationship : High												

Prepared by:

1. Dr. A. JAFAR AHAMED
2. Dr. M. SYED ALI PADUSHA

Checked by: Dr. M. SEENI MUBARAK

Semester	Code	Course	Title of the Course	Hours	Credits	Max. marks	Internal marks	External marks
II	20PCH2CC5	Core – V	ORGANIC REACTIONS, STEREOCHEMISTRY AND NATURAL PRODUCTS	6	5	100	25	75

Course Outcome:

1. Predict R, S and E, Z – notation in Organic compounds.
2. Categorize stereoselective and enantio selective asymmetric synthesis.
3. Differentiate aromatic, anti-aromatic and non-aromatic compounds.
4. Conclude the structure and importance of alkaloids, terpenoids, heterocyclic compounds and to appraise their medicinal properties.
5. Generate the mechanism for different types of novel synthetic methods.

UNIT-I

18 hours

Stereochemistry

1.1. #Newman, Sawhorse and Fisher projection formulae and interconversion#. Concept of chirality- Enantiotopic and diastereotopic atoms and groups, Prochirality, stereogenic centre and enantiomeric excess. E-Z nomenclature. Determination of configuration of geometrical isomers.

1.2. R, S notations of acyclic and cyclic chiral compounds - allenes, spiranes and biphenyl.

1.3. Conformational Analysis: Conformation of some simple 1, 2-disubstituted ethane derivatives. Conformation of cyclic compounds 3, 4, 5 & 6 membered rings. Conformational analysis of mono and di substituted cyclohexane and cyclohexanone. Stereochemistry of cis and trans decalin.

UNIT-II

18 hours

Asymmetric synthesis and Dynamic stereochemistry

2.1 Asymmetric Synthesis – Basic Principles – stereoselective reduction of cholestan-3-one (Diastereoselectivity), conversion of L-tyrosine into L-DOPA, nucleophilic attack on acyclic chiral carbonyl compounds (Cram's rule – the Felkin – Ahn modification, a diastereoselective synthesis, Enantioselective aldol condensation via chiral enolates (Double asymmetric synthesis) the use of chiral reagents (Third – generation method) and chiral catalysts, asymmetric reduction using chiral trialkylboranes (enantioselective reduction of aldehydes and ketones) asymmetric reduction using lithium aluminium hydride (reduction via chiral metal hydride complexes) use of Baker's yeast.

2.2. Dynamic stereochemistry: Quantitative correlations between conformation and reactivity. Weinstein-Eliel equation – Curtin-Hammett principle – Conformation and reactivity of mono and di substituted cyclic systems – Saponification of ester – Esterification of an alcohol – Chromic acid oxidation of cyclohexanol – Neighbouring group participation – De-amination of 2-amino cyclohexanol – Sharpless asymmetric epoxidation – stereospecific and stereoselective reactions.

UNIT-III

18 hours

Aromaticity

3.1. Definition of Aromaticity – Huckel's and Craig's Rules. Ring currents. Non-benzenoid aromatic compounds – Aromatic character in Three, Five, Six, Seven and Eight membered ring. Effect of aromaticity on bond lengths, resonance energies and induced ring current. Aromatic character in fused ring systems. Concept of Homo aromaticity and Hetero aromaticity.

3.2. Systems with Two, Four, Eight and Ten electron systems. Annulene. Aromaticity in Sydnones, Azulene and fullerenes. Alternant and non-alternant hydrocarbons.

UNIT-IV**18 hours****Heterocyclic Compounds, Terpenoids and Alkaloids**

4.1. Heterocyclic Compounds: Chemistry of non-aromatic heterocycles- Oxiranes, Thiranes, and Azetidines. Ring synthesis and reactions of aromatic heterocycles - Oxazoles, Thiazoles and Imidazoles,.

4.2. Terpenoids: Classification of Terpenoids - Structural elucidation and medicinal uses of α -Pinene, Camphor and Zingiberene.

4.3. Alkaloids: Classification of alkaloids- Structural elucidation and medicinal values of quinine, Papaverine and morphine.

UNIT-V**18 hours**

5.1. Name reactions: Dieckmanns, Stobbe, Darzen's Glycidic ester condensation, Houben -Hoesch. Vilmesmier-Haack and Knoevenagal

5.2. Concerted rearrangements: Cope (including Oxy-Cope) and Claisen.

5.3. Cationic rearrangements: Demjanov, Pummerer, Schmidt and Dienone -phenol.

5.4. Anionic rearrangements: Brook, Favorski, Neber, Von Richter, Sommelet - Hauser.

TEXT BOOKS:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1.	D.Nasipuri,	Stereochemistry of organic compounds – principles and Applications	2 nd Edition	New Age internationals	2002
2.	Ernest L. Eliel	Stereochemistry of Organic Compounds	1 st Edition	Wiley	2010
3.	P.S. Kalsi	Stereochemistry of organic compounds	8 th Edition	New Age internationals publishers private Limited	2010
4.	V.K. Ahluwalia & Rakesh K.Parashar	Organic Reaction Mechanism	4 th Edition	Narosa Publication	2010
5.	Gurdeep Chatwal	Organic Chemistry of Natural Products	5 th Edition	Himalaya Publishing House	2005

Books for Reference:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1	F.A. Carey and R.J. Sund berg	Advanced Organic Chemistry	Vol.I & II 3 rd Edition	Plenum Publications.	1984
2	S.P. Shukla and G.L Trivedi	Modern Organic Chemistry.	Millinium , 2 nd Edition	Rajendran Ravidra Printers Pvt.Ltd., New Delhi	2000

Web Reference: https://swayam.gov.in/nd1_noc19_cy25/preview

Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes:

Semester	Code	Title of the Paper					Hours	Credits			
II	20PCH2CC5	ORGANIC REACTIONS, STEREOCHEMISTRY AND NATURAL PRODUCTS					6	5			
Course Outcomes (COs)	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)					
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	
CO1	✓	✓		✓	✓	✓	✓			✓	
CO2	✓	✓		✓	✓	✓	✓			✓	
CO3	✓	✓		✓	✓	✓	✓			✓	
CO4	✓	✓	✓	✓	✓	✓	✓		✓	✓	
CO5	✓	✓		✓	✓	✓	✓		✓	✓	
Number of Matches = 38, Relationship : High											

Prepared by:

1. Dr. J. Sirajudeen
2. Dr. J. Muneer Ahamath

Checked by: Dr. M. Mohamed Sihabudeen

Semester	Code	Course	Title of the Course	Hours	Credits	Max. marks	Internal marks	External marks
II	20PCH2CC6	Core – VI	THEORY AND APPLICATIONS OF GROUP THEORY AND SPECTROSCOPY	6	5	100	25	75

Course outcome:

1. Construct the character table for molecules of different point groups.
2. Appraise spectroscopic selection rules to molecules applying group theoretical concepts.
3. Differentiate molecular symmetry and crystallographic symmetry.
4. Apply the theory of IR and Raman spectroscopy.
5. Compare the principles and applications of NMR, NMRI and solid state NMR.

UNIT – I

18hours

Elements of Group Theory

- 1.1 Symmetry elements and symmetry operations, Group - Rules for forming a Group, Finite Group, Infinite Group, Abelian Group, Cyclic Group, Sub Groups, Group Multiplication Table- Class and Similarity transformation.
- 1.2 Point Group – Method of Assigning Point Group- Schoenflies symbols, derivation of Matrix form of E , C_n , σ , S_n and i . Reducible and Irreducible Representations.
- 1.3 The Great Orthogonality Theorem – Properties of Irreducible Representation, Construction of Character Table for C_{2v} , C_{2h} and C_{3v} point Groups – Explanation of Character Table- basic idea of correlation table.

UNIT – II

18hours

Applications of Group Theory -I

- 2.1 The direct product and its applications, applications of group theory to spectroscopy – vanishing of integrals, symmetry selection rules for vibrational, Raman and electronic spectroscopy.
- 2.2. Reduction Formula and its applications, determination of symmetries of vibrational modes and their IR and Raman activities in non-linear molecules (H_2O , NH_3 and BF_3) and linear molecules (CO_2 and C_2H_2) sub group and Integration method, mutual exclusion rule, electronic transitions in formaldehyde and ethylene using group theory.

UNIT – III

18hours

Applications of Group Theory -II

- 3.1 Applications of Group theory - Hybridization schemes for atoms in molecules of different geometry – tetrahedral (CH_4), triangular (BF_3) planar linear (C_2H_2) and non-linear (C_2H_4) molecules.
- 3.2 Symmetry in crystals - Hermann - Mauguin symbols. Space groups of crystals - Translational elements of symmetry - Comparison of crystal symmetry with molecular symmetry.
- 3.3 Projection Operator – Symmetry Adapted Linear Combination (SALC) procedure. Symmetry factors of secular determinant and its applications to butadiene.

UNIT – IV

18 hours

Theory of IR and Raman Spectroscopy

- 4.1 IR Spectra- Theory of Rotational-Vibrational spectra – Harmonic and anharmonic oscillator. Calculation of force constant and effect of isotopic substitution on vibrational frequencies. Hot band, overtones, Fermi resonance, combination bands. Coupling of rotation and vibration-linear and perpendicular bands – PQR branches – (Problems - force constant)

4.2. **Raman Spectra-** #Polarization of light and Raman Effect– elastic and inelastic scattering.# Pure rotational and rotational-Vibrational Raman spectra. Lasers-special properties of laser, types of lasers. Laser Raman spectroscopy- theory and its advantages. Resonance Raman Spectroscopy, surface enhanced Raman scattering-theory and advantages.

UNIT – V

18hours

Theory of NMR Spectroscopy

5.1. Behavior of a bar magnet in a magnetic field – Magnetization vectors – resonance condition– relaxation process – effect of quadrupole nuclei on relaxation mechanism- Bloch equation–# chemical shift and its measurement#-

5.2. Scalar Spin - Spin Coupling Mechanism – Nature of the Coupling, Direct Dipolar Coupling –NMR in solids-Magic angle spinning- Nuclear Magnetic Resonance Imaging (NMRI) – principle and applications

5.3. FT-NMR – Principle, measurements of T1 by FTS, Use of T1 for peak assignment, Theory and advantages of 2D NMR

Self study

Text Books:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1.	K.V. Raman	Group theory and its Application to Chemistry	1 st Edition	Tata-McGraw –Hill Publishing Company Limited, New Delhi	2000
2.	K. Veera Reddy	Symmetry and Spectroscopy of Molecules	Reprint	New Age International Publishers	2010
3.	C. N. Banwell and E. M. Mccash,	Fundamentals of Molecular Spectroscopy	Fourth Edition (Indian Edition)	Tata McGraw-Hill Publishing Company Limited, New Delhi,	2017
4.	G. M. Barrow	Introduction to Molecular Spectroscopy	Revised Edition	Tata-McGraw- Hill Edition	1993

Books for Reference:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1.	F. A. Cotton,	Chemical Application of Group Theory	2 nd edition	Wiley – Eastern Press	1995
2.	G. Aruldas	Molecular Structure and Spectroscopy	2 nd Edition	PHI learning Pvt. Ltd., New Delhi	2016
3.	Manas Chanda	Structure and Chemical Bonding including Molecular Spectra	Reprint	Tata- McGraw-Hill Publishing company Ltd., New Delhi-2.	2000
5.	R. S. Drago	Physical Methods in Chemistry	Reprint	East West Press Ltd.,	1971

Web Reference:

Unit-I, II and III; www.nptel.ac.in/courses/104104080/

Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes:

Semester	Code	Title of the Paper					Hours	Credits				
II	20PCH2CC6	THEORY AND APPLICATIONS OF GROUP THEORY AND SPECTROSCOPY					6	5				
Course Outcomes (COs)	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)						
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5		
CO1	✓	✓				✓						
CO2	✓	✓	✓				✓			✓		
CO3	✓	✓	✓			✓						
CO4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		
CO5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		
Number of Matches = 32, Relationship : Moderate												

Prepared by:

1. Dr. M. SYED ALI PADUSHA
2. Dr. M. ANWAR SATHIQ

Checked by: Dr. M. SEENI MUBARAK

Semester	Code	Course	Title of the Course	Hours	Credits	Max. marks	Internal marks	External marks
II	20PCH2CC7P	Core – VII	INORGANIC QUALITATIVE ANALYSIS AND COLORIMETRIC ESTIMATIONS - PRACTICAL	6	4	100	25	75

Course Outcomes:

1. Analyse the elements in a mixture.
2. Categorize the metals based on its nature.
3. Spot a metal ion by carrying out a suitable reaction.
4. Apply the principle of photo colorimetry for metal ion estimation.
5. Appraise the principle of photo colorimetry in food product analysis

Semi-micro Qualitative Analysis: (50 Marks)

Analysis of two common and two rare earth elements in a given inorganic mixture

Common: Pb, Cu, Bi, Cd, Zn, Co, Ni, Ca, Ba, Sr

Rare: W, Se, Te, Mo, Ce, Zr, Th, V, Li

Colorimetric Estimations: (25 Marks)

Cu, Fe, Mn, Ni, Cr, **Viva-voce: (5Marks)**

Scheme of Valuation:

Procedure Writing - 10 Marks

Marks Viva - 10 Marks

Analysis:

4 radicals correct with suitable tests: 40 marks

3 radicals correct with suitable tests: 30 marks

2 radicals correct with suitable tests: 20 marks

1 radical correct with suitable tests: 10 marks

Colorimetric Estimations:

1-2% - 20 marks

2-3% - 15 marks

3-4% - 10 marks

>4% - 05 marks

Text Books:

S.No.	Author Name	Book Name	Edition	Publisher detail	Year
1.	Vogel A I	A Text Book of Quantitative Inorganic Analysis	3 rd Edition	Longman Group	1972

Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes:

Semester	Code	Title of the Paper	Hours	Credits						
II	20PCH2CC7P	INORGANIC QUALITATIVE ANALYSIS AND COLORIMETRIC ESTIMATIONS - PRACTICAL	6	4						
Course Outcomes (COs)	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓		✓		✓	✓			
CO2	✓	✓		✓		✓			✓	
CO3	✓	✓				✓	✓		✓	✓
CO4	✓	✓	✓			✓	✓	✓		
CO5	✓	✓		✓	✓	✓	✓		✓	✓
Number of Matches = 30, Relationship : Moderate										

Prepared by:

1. Dr.M.Syed Ali Padusha
2. Dr. F. M. Mashood Ahamed

Checked by:

Dr. A. Jamal Abdul Nasser

Semester	Code	Course	Title of the Course	Hours	Credits	Max. marks	Internal marks	External marks
II	20PCH2CC8P	Core – VIII	QUALITATIVE ANALYSIS OF ORGANIC MIXTURE AND CHROMATOGRAPHY TECHNIQUES - PRACTICAL	6	4	100	25	75

Course Outcomes:

1. Apply pilot separation technique to the organic compounds based on the solubility
2. Examine the components present in the given organic mixture by carrying of specific reactions
3. Identify the functional group present in the components
4. Understand the concept of TLC techniques and record the R_f value of given amino acids
5. Apply thin layer chromatography techniques for the separation of amino acids

Identification of components in a two component mixture: 60 Marks

Mixture containing two components are to be separated (pilot separation) and purified (bulk separation). Separate the following types of mixture and analyze only one of the components present as desired by the Teacher / Examiner.

Mixture Analysis:

1. Soluble and insoluble
2. Acidic and neutral
3. Less acidic and neutral
4. Basic and neutral

Chromatographic Technique 15 Marks

Separation of amino acid mixture by Thin Layer Chromatography

Viva-voce: 05 Marks

Scheme of Valuation:

Organic Analysis - 60 marks

Organic Analysis:

Procedure Writing - 10 marks
Pilot separation - 10 marks
Special elements present / absent - 08 marks
Aromatic/ aliphatic - 08 marks
Saturated/ unsaturated - 08 marks
Functional group present - 08 marks
Derivative - 08 marks

Chromatographic Technique - 15 Marks

Text Books:

S.No.	Author Name	Book Name	Edition	Publisher detail	Year
1.	Vogel A I	A Text Book of Practical Organic Analysis	5 th Edition	Longman Group	1989

Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes:

Semester	Code	Title of the Paper	Hours	Credits						
II	20PCH2CC8P	QUALITATIVE ANALYSIS OF ORGANIC MIXTURE AND CHROMATOGRAPHY TECHNIQUES - PRACTICAL	6	4						
Course Outcomes (COs)	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓		✓		✓	✓			✓
CO2	✓	✓				✓	✓	✓		
CO3	✓	✓			✓	✓	✓	✓		
CO4	✓	✓		✓		✓	✓	✓		✓
CO5	✓	✓		✓	✓	✓	✓			✓
Number of Matches = 31, Relationship : Moderate										

Prepared by:

1. Dr. A. Zahir Hussain
2. Dr. A. Asrar Ahamed

Checked by: Dr. M. Mohamed Sihabudeen

Semester	Code	Course	Title of the Course	Hours	Credits	Max. marks	Internal marks	External marks
II	20PCH2DE2A	DSE – II	CHEMISTRY OF COMPLEXES AND ORGANOMETALLICS, IR, ELECTRONIC AND MOSSBAUER SPECTROSCOPY	6	4	100	25	75

Course Outcomes:

1. Examine the stability of complexes and to apply various reactions of coordination compounds in their research.
2. Design the synthesis, structure and bonding of carbon π -acceptor and donor complexes.
3. Apply the different type of organometallic reactions to explain different catalytic reactions.
4. Sketch the electronic transition in various d^n -systems.
5. Apply various spectroscopic principles to characterise inorganic and organometallic compounds

UNIT-I

18 hours

1.1. Reactivity of Complexes in solutions – Labile and inert complexes. Ligand displacement reactions – hydrolysis, acid, base and aquation in O_h complexes. Electron Transfer Reactions - complementary and non-complementary, inner and outer sphere processes. Isomerism in square planar complexes. Trans effect – Theories and its applications. Template effect.

1.2. Stability of coordination compounds: Detection of complex formation in solution-stability constants, stepwise, overall formation constants, determination by pH-metric, polarographic and photometric methods. Factors affecting stability - statistical and chelate effects.

UNIT– II

18 hours

Complexes of π acceptor and donor ligands

2.1. Carbonyls - $18e^-$ rule, applications of $18e^-$ rule to structural study of poly nuclear carbonyls, carbonylate anions, carbonyl hydrides, isolobal fragments. Nitrosyl complexes – Preparation and structure of bridging and terminal nitrosyls, bent and linear nitrosyls. Dinitrogen and dioxygen complexes.

2.2. Carbon π -donor Complexes: Synthesis, structure and bonding of alkene (Zeise's salt), alkyne and allyl complexes. Metallocenes-Ferrocene, preparation, properties and structure (Molecular orbital concept).

UNIT– III

18 hours

3.1. Organometallic Chemistry: Ligand association and dissociation – oxidative addition and reductive elimination – insertion reactions – Catalysis by Organometallics - Hydrogenation, hydroformylation, polymerisation of alkenes, olefin oxidation (Wacker Process), Fischer–Tropsch synthesis, epoxidation, metathesis.

3.2. Metallobiomolecules: Hemoglobin and myoglobin – Structure and functions (oxygen transport and storage). Electron transfer and oxygen activation - Ferredoxins and rubredoxins, copper proteins - oxidases and reductases, cytochrome oxidase, superoxide dismutase. [#]Urease and hydrogenases – structure and functions[#].

UNIT– IV**18 hours**

4.1. Electronic spectroscopy: Electronic configuration - Terms, states and microstates of atoms and ions – Derivation of term symbols d^n and arranging the various term according to their energies - spectroscopic terms – L-S coupling and jj coupling – # Racah parameters B and C – selection rules and the breakdown of selection rules – mixing of orbitals#.

4.2. Orgel diagram – characteristics, prediction and assignment of transitions for d^n weak field systems, band intensity, band width, band shape, calculation of β and $10 Dq$ for simple octahedral complexes of Co and Ni. Tanabe-Sugano diagrams – prediction and assignment of transitions for weak field and strong field of d^n systems. Charge transfer spectra - LMCT and MLCT.

UNIT– V**18 hours**

5.2. IR and Raman spectroscopy: Combined uses of IR and Raman spectroscopy in the structural elucidation of N_2O , H_2O , ClF_3 , NO_3^- and ClO_3^- . Effect of coordination on ligand vibrations. Uses of group vibrations in the structural elucidation of metal complexes of urea, cyanide, nitrate and sulphate. Effect of isotopic substitution on vibrational spectra of metal carbonyls.

5.3. Mossbauer Spectroscopy: Mossbauer transition and Doppler Effect - isomer Shift, quadrupole effect – application to iron and tin compounds.

5.4. Lanthanides and Actinides: Co-ordination compounds of lanthanides and actinides, spectral and magnetic properties. #synthesis of transuranic elements#.

#_____# Self-study portion

TEXT BOOKS:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1	R.Gopalan, V.Ramalingam	Concise Coordination Chemistry	-	Vikas Publishing House Pvt. Ltd., Newdelhi	2001
2	B.D.Gupta, A.J.Elias	Basic Organometallic Chemistry-Concepts, Syntheses and Applications	-	University Press, Hyderabad	2011
3	R.C.Mehrotra, A.Singh	Organometallic Chemistry-A Unified Approach	Revised 2 nd Edition	New Age International Publishers	2011
4.	Satya Prakash, G.D.Tuli, S.K.Basu, R.D.Madan,	Advanced Inorganic Chemistry Vol-I	-	S.Chand & Co., Ltd., New Delhi.	2011

Books for Reference:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1.	Cotton and Wilkinson	Advanced Inorganic Chemistry	6 th Edition	John Wiley & Sons, New York	2004
2.	James E. Huheey, Ellen A. Keiter and Richard L. Keiter	Inorganic Chemistry Principles of Structure and Reactivity	4 th Edition	Pearson Education, 11 th Impression	2011
3.	R.H. Crabtree	The Organometallic Chemistry of the Transition Metals:	-	John Wiley & Sons, New York	2000
4.	W. Kaim and B. Schwederski	Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life:	-	John Wiley & Sons, New York, USA	2001
5.	P.Powell	Principles of Organometallic Chemistry	-	2 nd Edn.: Chapman and Hall, London	2003

Web Reference: https://nptel.ac.in/content/syllabus_pdf/104101121.pdf

Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes:

Semester	Code	Title of the Paper	Hours	Credits						
II	20PCH2DE2A	CHEMISTRY OF COMPLEXES AND ORGANOMETALLICS, IR, ELECTRONIC AND MOSSBAUER SPECTROSCOPY	6	4						
Course Outcomes (COs)	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓		✓	✓	✓	✓		✓	✓
CO2	✓	✓		✓	✓	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO4	✓	✓		✓	✓	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Number of Matches = 46, Relationship : High										

Prepared by:

- 1.Dr.K. Loganathan
- 2.Dr.N. Mujafarkani

Checked by: Dr.A.Jamal Abdul Nasser

Semester	Code	Course	Title of the Course	Hours	Credits	Max. marks	Internal marks	External marks
II	20PCH2DE2B	DSE – II	SPECTROSCOPY OF INORGANIC COMPLEXES AND ORGANOMETALLICS	6	4	100	25	75

Course Outcomes:

1. Sketch the electronic transition in various d^n -systems
2. Apply various spectroscopic principles to characterise inorganic and organometallic compounds
3. Design various processes in extraction of metals and manufacture of alloys.
4. Examine the stability of complexes and to apply various reactions of coordination compounds in research.
5. Apply the different type of organometallic reactions to explain different catalytic reactions.

UNIT– I

18 hours

- 1.1 **Electronic spectroscopy:** Electronic configuration - Terms, states and microstates of atoms and ions – Derivation term symbols (p^2 and d^2) and arranging the various term according to their energies spectroscopic terms – L-S coupling and JJ coupling – #effect of interelectronic repulsion and spin-orbit coupling# – Racah parameters B and C – selection rules and the breakdown of selection rules – mixing of orbitals.
- 1.2 Orgel diagram – characteristics – prediction and assignment of transitions for dn weak field systems. Tanabe – Sugano diagrams – prediction and assignment of transitions for weak field and strong field – d^n systems band intensity, band widths- band shapes- calculation of β and $10 Dq$ for simple octahedral complexes of Co and Ni- charge transfer spectra.

UNIT– II

18 hours

- 2.1 **IR and Raman spectroscopy:** Combined use of IR and Raman spectroscopy in the structural elucidation of N_2O , H_2O , ClF_3 , NO_3^- , ClO^- - Effect of coordination on ligand vibrations – uses of group vibrations in the structural elucidation of metal complexes of urea, cyanide, nitrate and sulphate – #Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal complexes#.
- 2.2 **Mossbauer Spectroscopy:** Mossbauer transition and Doppler Effect – isomer shift quadrupole effect – magnetic effect on spectra – simple application to iron and tin compounds.
- 2.3 **Lanthanides and Actinides:** co-ordination compounds of lanthanides- spectral and magnetic properties of Lanthanides and Actinides, synthesis of transuranic elements

UNIT– III

18 hours

- 3.1 **Extraction and Uses of Metals:** Metallurgy of Zr, Ge, Th and U –#uses of their important compounds.#
- 3.2 **Alloys and Intermetallic Compounds** – Effect of alloying – types of alloys – simple mixtures – solid solutions – substitutional alloys – Industrial alloys – Substitutional alloys - Intermetallic Compounds – Hume – Rotherys rules – ferrous alloys , non- ferrous alloys – Al, Mg alloys, amalgams, alloy steels.
- 3.3 **Inorganic Polymers and Rings:** Phosphorus based network polymers, Coordination Polymers (Structure and properties). Preparation and Structure of Borazines & Phosphazenes Craig and Paddock model - Dewar model – Preparation and Structure of sulphur-nitrogen ring system (S_4N_4 , $N_4S_4F_4$)

UNIT– IV**18 hours**

- 4.1 **Reactivity of Complexes** – Kinetics and Mechanisms of reactions in solutions: Labile and inert complexes – Ligand displacement Reactions – hydrolysis – acid & base, aquation in O_h complexes. Electron Transfer Reactions, complementary and non-complementary types – inner and outer sphere processes – Isomerism in square planar complexes – Trans effect – Theories and Applications. Template effect and synthesis of macrocyclic ligands.
- 4.2 **Stability of coordination compounds:** Detection of complex formation in solution, stability constants, stepwise and overall formation constants pH metric, #polarographic and photometric methods of determining formation constants# - factors affecting stability – statistical and chelate effects.

UNIT– V**18 hours**

- 5.2 **Organometallic Chemistry:** 16 and 18 electron rule - Catalysis by Organometallics- Ligand association and dissociation – oxidative addition and reductive elimination – insertion reactions – reactions of coordinated ligands in organometallics – Hydrogenation, hydroformylation, polymerisation of alkenes, olefin oxidation (Wacker Process), Fischer–Tropsch synthesis, epoxidation, metathesis.
- 5.3 **Oxygen Transport and energy transfer of metals proteins:** # Hemoglobin and myoglobin – Oxygen transport and storage#. Electron transfer and Oxygen activation. Ferredoxins and rubredoxines – Copper proteins – classification – Electron transfer, oxygen transport. Oxidases and reductases – cytochrome oxidase – superoxide dismutase (Cu, Zn), Urease and hydrogenases.

_____# Self-study portion

TEXT BOOKS:

S. No.	Author Name	Book Name	Edition	Publisher detail	Year
1	R.Gopalan and V.Ramalingam	Concise Coordination Chemistry	1 st edition	Vikas Publishing House Pvt. Ltd., New Delhi	2001
2	B.D.Gupta and A.J.Elias	Basic Organometallic Chemistry-Concepts, Syntheses and Applications	-	University Press, Hyderabad	2011
3	R.C.Mehrotra and A.Singh	Organometallic Chemistry-A Unified Approach”	Revised 2 nd edition	New Age International Publishers	2011
4.	G D Tuli, S K Basu, Satya Prakash and R D Madan	Advanced Inorganic Chemistry Vol-I	19 th edition	S.Chand & Co., Ltd., New Delhi	2016
5.	Wolfgang Kaim, Brigitte Schwederski and Axel Klein	Bioinorganic Chemistry -- Inorganic Elements in the Chemistry of Life: An Introduction and Guide	2 nd Edition	John Wiley & Sons,	2013

Books for Reference:

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2.	Cotton and Wilkinson	Advanced Inorganic Chemistry	6 th Edition	John Wiley & Sons, New York	2004
3.	Gurdeep raj	Advanced Inorganic Chemistry-Vol.-I	-	Krishna's Educational Publishers	2014
4.	R.H. Crabtree	The Organometallic Chemistry of the Transition Metals	-	John Wiley & Sons, New York	2000
5.	E.A.V. Ebsworth, W.H. Rankin, Cradock	Structural Methods in Inorganic Chemistry	-	ELBS	1987

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Relationship Matrix for Course Outcomes, Programme Outcomes and Programme Specific Outcomes:

Semester	Code	Title of the Paper	Hours	Credits						
II	20PCH2DE2B	SPECTROSCOPY OF INORGANIC COMPLEXES AND ORGANOMETALLICS	6	4						
Course Outcomes (COs)	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓		✓	✓	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓	✓	✓		✓	✓
CO3	✓	✓		✓	✓	✓	✓	✓	✓	✓
CO4	✓	✓		✓	✓	✓	✓	✓	✓	✓
CO5	✓	✓	✓		✓	✓	✓	✓	✓	✓
Number of Matches = 40, Relationship : High										

Prepared by:

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