Sacred Heart College (Autonomous), Tirupattur District

1.2.1 List of New Courses

M.Sc. Chemistry (CBCS)

Sem	Sub	Title of the paper	Ins Hrs	Cr	CA Mks	Sem Mks	Total
I	Core	Organic Chemistry – I	4	4	50	50	100
	Core	Inorganic Chemistry – I	4	4	50	50	100
	Core	Physical Chemistry – I	5	4	50	50	100
	Core Practicals	Organic Practicals – I	4	-	-	-	-
		Inorganic Practicals – I	4	-	-	-	-
		Physical Practicals – I	4	-	-	-	-
	Elective - I	1. Analytical Chemistry 2. Green Chemistry 3. Pharmaceutical Chemistry	5	5	50	50	100
II	Core	Organic Chemistry – II	4	4	50	50	100
	Core	Inorganic Chemistry – II	4	4	50	50	100
	Core	Physical Chemistry – II	5	4	50	50	100
	Elective - II	1. Research Methodology 2. Heterocyclic Chemistry 3. Bio-organic Chemistry	5	5	50	50	100
	SSP	Reagents in Organic Chemistry	0	2*			
	Core Practicals	Organic Practicals – I	4	4	50	50	100
		Inorganic Practicals – I	4	4	50	50	100
		Physical Practicals – I	4	4	50	50	100
III	Core	Organic Chemistry – III	4	4	50	50	100
	Core	Inorganic Chemistry – III	4	4	50	50	100
	Core	Spectroscopy	5	4	50	50	100
	Elective - III	1. Inorganic photochemistry and materials science 2. Polymer Chemistry 3. Chemoinformatics	5	5	50	50	100
	Core Practicals	Organic Practicals – II	4	-	-	-	-
		Inorganic Practicals – II	4	-	-	-	-
		Physical Practicals – II	4	-	-	-	-
IV	Core	Organic Chemistry – IV	4	4	50	50	100
	Core	Inorganic Chemistry - IV	4	4	50	50	100

	Core	Physical Chemistry – III	5	4	50	50	100
	Core Practicals	Organic Practicals – II	4	4	50	50	100
		Inorganic Practicals – II	4	4	50	50	100
		Physical Practicals – II	4	4	50	50	100
	HR	Human Rights	2	1	50	50	100

	Project	Project Work	3	2	20 Viva	80 Thesis	100
	IDC	Advanced analytical technique/BMT		2*			
	SSP	Chemical Sciences For CSIR-UGC–NET/JRF/ GATE		2*			
		Total	**120**	**90+6***			**2200**

Required Credits = 90 (89 + 1–HR)

<u>Additional credits for Chemistry students</u> - 6* Credits

1. Credits from parent department (2+2)

Self-Study Paper (Chemical Science for CSIR/SET) : 2* Credits
Self-Study Paper (Reagents in Organic Chemistry) : 2* Credits

2. Additional credits (Chemistry, Bio-chemistry and Physics department)

Inter Disciplinary Course (IDC) : 2*Credits

Advanced Analytical Techniques / BMT

- **Classes will be taught outside the class hours**
- **Based on the demand the course fee may be fixed**

Regulations for Inter Disciplinary Course [IDC]

IDC- AAT / Biochemical and Microbial Techniques

Credit : 2*Credits
Hours : 30 Hours (20+10)
Semester : II Year [Semester - III & IV]
Evaluation Pattern : Test-I and Test-II
Maximum Marks : 50 Marks
Minimum Marks : 25 Marks

Regulations for Self-Study Paper [SSP]

1. Reagents in organic Chemistry
2. Chemical Science for CSIR / SET

Credit : 2*Credits
Semester : Semester - II and IV
Evaluation Pattern : one Test
Maximum Marks : 100 Marks
Minimum Marks : 50 Marks

Sacred Heart College (Autonomous), Tirupattur District

1.2.1 List of New Courses

Department: M.Sc.Chemistry

S.No	Course Code	Course Name
1.	CH918	Organic Chemistry - III
2.	CH919	Inorganic Chemistry - III
3.	CH920	Spectroscopy
4.	CH921A	Elective-III Inorganic Photochemistry and Materials Science
5.	CH921B	Elective-III Polymer Chemistry
6.	CH921C	Elective-III Cheminformatics
7.	CH1017	Organic Chemistry - IV
8.	CH1018	Inorganic Chemistry - IV
9.	CH1019	Physical Chemistry - III
10.	PCH1013	Organic Practicals - II
11.	PCH1014	Inorganic Chemistry-II
12.	PCH1015	Physical Chemistry Practicals

Syllabus:

SEMESTER-II

Organic Chemistry III

Course Code	**CH918**	**Credit**	**4**
Instruction Hours per Week	**4**	**Marks**	**CIA (50) / SE (50)**
Course Objective	• To learn photochemical reactions, pericyclic reactions and their importance. • To learn the synthetic application of Organometallic compounds.		

Course Outcomes:

Sl. No.	**Course Outcome Statements**	**Knowledge level**
	On successful completion of this Course, students will be able to	
CO1	Identify the nature of rearrangement involved and intermediates generated in various organic molecules; Writing mechanism for the rearrangement involved in organic molecules.	**K1, K6**
CO2	Interpret the role of reagents in multistep organic synthesis and correlate the next synthetic work up involved.	**K2**
CO3	Integrate the concept of organometallic compounds as homogeneous, hetereogeneous catalysts and reagents in organic functional group conversions.	**K3**
CO4	Illustrate list of electronic transitions involved in various organic molecules and correlate them with photochemical reactions and based on their photophysical processes.	**K4**
CO5	Invent corresponding mechanism based on thermal/photochemical condition and predicting the product with specific stereochemistry in various pericyclic reactions.	**K5**
CO6	Build the synthetic route theoretically for a given reactant and product with set of reagents.	**K6**

Mapping of CO with PO and PSO

CO	Programme Specific Outcomes (PSO)						Programme Outcomes (PO)					Mean Scores of COs
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PO1	PO2	PO3	PO4	PO5	
CO1	3	2	3	2	2	1	3	3	3	3	1	2.3636364
CO 2	3	2	3	1	2	1	3	2	1	3	1	2
CO 3	3	2	3	3	2	2	3	3	2	3	2	2.5454545
CO 4	3	3	3	2	1	2	3	3	1	2	1	2.1818182
CO 5	3	2	3	1	1	2	2	2	1	3	2	2
CO 6	3	2	3	2	3	2	3	3	2	3	2	2.5454545
											Mean Overall Score	2.272727
											Result	

Assessment Pattern

Bloom's Category	CA Tests (Marks Allotment)		Term End Exam (100) Marks Allotment
	I CA (50)	II CA (50)	
Remember	10	10	20
Understand	10	10	30
Apply	10	10	20
Analyze	10	10	10
Evaluate	5	5	10
Create	5	5	10

Course Content

Unit - I: Molecular Rearrangements **12 Hours**

Types of rearrangements: Nucleophilic; free radical and electrophilic reactions. Mechanisms: Nature of migration; migratory aptitude and memory effects, ring enlargement and ring contraction rearrangements Reactions: Wagner-Meerwin and related reactions, Benzil-benzilic acid, Favorskii, Hofmann and related rearrangements, Beckmann, Neber, Baeyer-Williger, Stevens, boron-carbon migration, Non-1,2-rearrangements, Fischer-indole synthesis, Arndt-Eistert synthesis

Unit - II: Reagents in Organic Synthesis **12 Hours**

Enammine chemistry and its synthetic applications,aluminiumIsopropoxide, DCC, *n*-BuSnH, baker yeast, Woodward and Prevost dihydroxylations, NBS, DDQ, LTA, LDA , wilkinson's catalyst, and Diazomethane, wittig Reagent, Gilman reagent, Corey's reagent, Merrifield reagent.

Unit - III: Synthetic Applications of Organometallic Compounds 12 Hours

Synthesis and applications of organoboranes – Grignard reagents - organomercury compounds – aromatic mercuration, organolithium compounds - organothallium compounds - organocopper compounds, organolead compounds and organoaluminium compounds.

Unit - IV: Organic Photochemistry 12 Hours

Introduction- Photochemical laws-electronic transitions- photochemistry of excited molecule-physical processes-photochemistry of carbonyl compounds- Norrish type I and II reactions- Hydrogen abstraction- photocycloaddition-Paterno – Buchi reactions- photorearrangement of cyclopentenone, cyclohexenone-Lumiketone rearrangement-photorearrangement of β,γ-unsaturated ketones-di- π-methane rearrangement-Aza- di- π-methane rearrangements-Analysis of cis-trans isomerisations

Unit - V: Pericyclic Reactions 12 Hours

Introduction to pericyclic reaction - Characteristics-types-applications of FMO and MO correlation diagram methods to electrocyclic and cycloaddition reactions- Woodward-Hoffmann rules and their applications to simple systems-cycloadditions involving hydrogen transfer- Analysis of Cycloaddition and Diels –Alder reactions, Detail study of Sigmatropic reactions- Cope and Claisenrearrangements,Chelotropicreaction,Group transfer reactions,Ene and retro enereactions,Coarctate reaction.

References

1. Clayden, Greeves, Warren and Wothers, Organic chemistry, Oxford University press, 2001.
2. Francis A Carey and Richard J. Sundberg, Advanced organic chemistry, 4thEdn., part B, 2001.
3. I.L. Finar, Organic Chemistry V Edition, Vol :ll ELBS Publication, 1986.
4. J. March, Advanced Organic Reaction mechanism and structure, Tata McGraw Hill, 2000.
5. Jagadamba Singh and Jaya Singh, Photochemistry and Pericyclic reactions, 3r^{d}edn., New Academic Science, 2012.
6. K. K. Rohatji Mukherjee, Fundamentals of photochemistry, 1st, edn., New Age Publications, 2008.
7. S. H. Pine, *Organic Chemistry*, 5thedn, McGraw Hill International Edition, 1987.
8. L. F. Fieser and M. Fieser, *Organic Chemistry*, Asia Publishing House, Bombay, 2000.
9. E.S. Gould, *Mechanism and structure in organic chemistry*, Holt, Rinehart and Winston Inc.,1959.

Online Resources

http://eacharya.inflibnet.ac.in/ Organic chemistry and pericyclic reactions [40 lectures]

Syllabus:

SEMESTER-III

Inorganic Chemistry-III

Course Code	**CH919**	**Credit**	**4**
Instruction Hours per Week	**4**	**Marks**	**CIA (50) / SE (50)**
Course Objective	• To study about the basic theory of Inorganic spectroscopy. • To illustrate the UV, IR and Raman spectral properties of some inorganic compounds and complexes. • To study and illustrate the different types of magnetic behaviour in inorganic materials. • To learn the basic concepts of superconductivity behaviour in the materials • To apply the NMR, NQR, ESR and Mossbauer techniques in to simple inorganic systems. • To learn the instrumentation of advance inorganic spectroscopy techniques.		

Course Outcomes

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

S. NO	Course Outcomes Statement	Cognitive level
CO1	Students can recognize and interpret the spectroscopic techniques in terms of interaction of electromagnetic radiation with molecules	**K1 & K2**
CO2	Students can infer about the magnetic properties and superconductivity of materials and can able to calculate the magnetic susceptibility of the materials.	**K2, K3 & K4**
CO3	Students can describe the principles and to interpret the instrumentation of various spectroscopic techniques.	**K1 & K3**
CO4	Students can illustrate the principle involved in ESR, NQR and Mossbauer Spectroscopy and distinguish chemical species using these spectroscopy	**K2 & K4**
CO5	Students can apply the principles of spectroscopy to predict the structure of compounds and analyse the various spectra of complexes	**K3, K4 &K5**
CO6	Students can able to propose and formulate the structure of a new compound based on the spectroscopic data	**K6**

Mapping of CO with PO and PSO

CO	Programme Specific Outcomes (PSO)						Programme Outcomes (PO)					Mean Scores of COs
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PO1	PO2	PO3	PO4	PO5	
1	3	3	3	3	2	2	3	3	2	2	3	2.6
2	3	3	3	3	3	2	3	3	3	3	2	2.8
3	3	3	3	3	3	3	3	3	3	3	2	2.9
4	3	3	3	3	3	2	3	3	3	3	2	2.8
5	3	3	3	3	3	3	3	3	3	3	2	2.9
6	3	3	3	3	3	3	3	3	3	3	2	2.9
Mean Overall Score												2.8
Result												**High**

Assessment Pattern

Bloom's Category	CA Tests (Marks Allotment)		Term End Exam (100) Marks Allotment
	I CA (50)	II CA (50)	
Remember	10	10	20
Understand	10	10	30
Apply	10	10	20
Analyze	10	10	10
Evaluate	5	5	10
Create	5	5	10

Course Content

Unit - I: Inorganic Spectroscopy - I and Magnetic Susceptibility 12 Hours

Applications to inorganic systems of the following: ultra violet, visible, infra-red and Raman spectra of metal complexes, organometallic and simple inorganic compounds with special reference to coordination sites, isomerism. Magnetic Susceptibility and measurements - Guoy method, Faraday method; applications.

Unit - II: Magnetic Properties and Superconductivity 12 Hours

Magnetic properties – classification - diamagnetic, paramagnetic, antiferromagnetic, ferro and ferri magnetic — magnetic susceptibility, Variation with temperature – Curie-Wiess law, Curie temperature and Neel temperature. Permanent and temporary magnets. Superconductivity – introduction, Meissner effect – mention of Bardeen, Cooper and Schrieffer theory and Cooper pairs – examples of superconducting oxides.

Unit - III: Inorganic Spectroscopy – II 12 Hours

Application to Inorganic systems of the following: NMR, NMR of 31P, 19F, NMR shift reagents, NQR introduction and NQR - Nitrosyl compounds. Mossbauer spectra – Theory and Mossbauer spectra of Fe and Sn systems.

Unit - IV: Inorganic Spectroscopy – III 12 Hours

ESR Introduction - Zeeman equation, g-value, nuclear hyperfine splitting, interpretations of the spectrum, simple carbon centered free radicals. Anisotropy - g-value and hyperfine splitting constant. McConnell's equation, Kramer's theorem. ESR of transition metal complexes of copper, manganese and vanadyl complex. Applications of ESR spectroscopy.

Photoelectron spectroscopy (UV and X-ray) - photo electron spectra - Koopman's theorem, time structure in PES, chemical shift and correlation with electronic charges.

Unit - V: AAS and ICP –AES 12 Hours

Atomic absorption spectroscopy- principle- Advantages and disadvantages of AAS. Instrumentation of AAS, Interferences in AAS - Applications of AAS – Determination of Mg in water and Lead in Petrol- principle of plasma spectroscopy - ICP-AES instrumentation - limitations of flame emission spectroscopy - applications of plasma spectroscopy - comparison of ICP-AES with AAS.

Text Books

References

1. C.N.R. Rao, I.R. Ferraro, Spectroscopy in Inorganic Chemistry, Vol. I and Vol. II, Academic Press, 1970.
2. G. Aruldhas, Molecular Structure and Spectroscopy – Prentice Hall, 1986.
3. D. A. Skoog and D.M.West, Principles of Instrumental Methods of analysis, Saunder's College Publ. III Edition, 1985.
4. E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, Structural Methods in Inorganic Chemistry, II Edition, Blackwell Scientific Publications, Oxford, London 1991.
5. G.D. Christian and J.E.G. Reily, Instrumental Analysis, AllegnBecon, II Edition, 1986.
6. H.A. Strobel, Chemical Instrumentation, Addison - Wesley Pub. Co., 1976.
7. R. S. Drago, Physical Methods for Chemists, Saunders College Publishing, Philadelphia 1992.
8. R.S. Drago, Physical methods in inorganic Chemistry, Reeindhod, NY, 1968.
9. Willard Merrit, Dean and Settle, Instrumental methods of analysis, CBS Publ. VI edition, 1986.
10. A.I Vogel, Text books of qualitative analysis, ELBS Editions, 1976 and IV Edition 1985.

Syllabus:

SEMESTER-II

CH920 – SPECTROSCOPY

Course Code	**C327**	**Credit**	**4**
Instruction Hours per Week	**4**	**Marks**	**CIA (50) / SE (50)**
Course Objective	• To understand the concepts of spectral techniques • To apply these techniques for the quantitative and structural analysis of organic compounds		

Course Outcomes

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

CO. No.	**Course Outcome Statement**	**Cognitive Level**
CO 1	Demonstrate the understanding of electromagnetic spectrum and applied to study of chemical molecules.	K1, K2
CO 2	Validate knowledge of the principles of mass spectrometry and instrumentation.	K2, K5
CO 3	Predict number of signals, splitting pattern in the proton NMR of a compound and interpret NMR spectra of simple molecules.	K3, K5
CO 4	Identify the absorption frequencies of major functional groups and comprehend the electronic absorption and apply to interpret IR and UV-Visible spectra of simple organic compounds.	K2, K4
CO 5	Develop an ability for combined usage of mass spectrometry, UV-Vis., IR and NMR for structural elucidation.	K3, K6
CO 6	Analyse, evaluate and interpret the spectroscopic data effectively	K4, K5

Mapping of CO with PO and PSO

CO	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)						
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	Mean Scores of COs
CO1	3	3	3	3	2	3	3	2	3	3	3	2.82
CO2	3	3	2	3	2	3	3	3	2	3	3	2.73
CO3	3	3	3	3	2	3	3	3	3	3	2	2.82
CO4	3	3	3	3	2	3	3	2	3	3	3	2.82
CO5	3	3	3	3	2	3	3	3	2	3	3	2.82
CO6	3	3	3	3	2	3	3	3	3	2	3	2.82
Mean Overall Score												2.80
Result												High

Assessment Pattern

Bloom's Category	CA Tests (Marks Allotment)		Term End Exam (100)
	I CA (50)	II CA (50)	Marks Allotment
Remember	10	10	20
Understand	10	10	30
Apply	10	10	20
Analyze	10	10	10
Evaluate	5	5	10
Create	5	5	10

Course Content

Unit - I: Elemental Analysis and Mass Spectra **15 Hours**

Calculation of empirical and molecular formula-Mass Spectroscopy – Principles – measurement techniques – (EI, CI, FD, FAB, SIMS) Molecular ions – isotope ions – fragmentations of odd and even electron types – rearrangement ions –factors affecting cleavage patterns – simple and multicentre fragmentation – McLafferty rearrangement. Mass spectra for various organic compounds- nitrogen rule.

Unit - II: UV –Visible Spectroscopy **15 Hours**

Ultraviolet – Visible spectroscopy – Instrumentation-single and double beam instruments-– types of electronic transitions – chromophores and auxochromes – factors influencing positions and intensity of absorption bands – absorption spectra of dienes, polyenes and unsaturated carbonyl compounds – Woodward – Fisher rules. Applications to simple systems.

Unit - III: Infra-Red Spectroscopy **15 Hours**

IR Spectroscopy – Selection rule- Instrumentation-Sample preparation-FTIR- vibrational frequencies and factors affecting them – identification of functional groups – intra and inter molecular hydrogen bonding – finger print region – Far IR region – metal ligand stretching vibrations.

Unit - IV: NMR **15 Hours**

Theory, Relaxation processes, spin – spin splitting Theory of Chemical Shift – Chemical exchange, Double Resonance techniques. Instrumentation - application to organic systems.

Nuclear spin – magnetic movement of a nucleus – nuclear energy levels in the presence of magnetic field relative populations of energy levels – macroscopic magnetization – basic principles of NMR experiments – CW and FT NMR –H NMR – Chemical shift and coupling constant – factors influencing proton chemical shift and vicinal proton – proton coupling constant - ^{1}H NMR spectra of simple organic molecules such as CH_3CH_2Cl, CH_3CHO etc. AX and AB spin system – spin decoupling – nuclear overhauser effect – chemical exchange.

Unit - V: ^{13}C NMR, ORD and CD **15 Hours**

^{13}C NMR – proton decoupled and off – resonance ^{13}C NMR spectra – factors affecting ^{13}C chemical shift - ^{13}C NMR spectra of simple organic molecules- elementary idea about 2D NMR- COSY-NOSEY-DEPT90 and 135. (Combined problem)

Optical rotatory dispersion and circular dichroism: Introduction to theory and terminology – cotton effect – ORD curves – axial haloketone rule and its applications – octant rule – its applications – applications of ORD to determine absolute configuration of monocyclic ketones – comparison between ORD and CD – their inter relationships.

References

1. J. Dyer, Application of absorption spectroscopy of organic compounds, Prentice and Hall of India, Pvt., New Delhi.1991.
2. R.M. Silvarstein, G.d. Bassler and Monsu. Johr, Spectrometric identification of organic compounds by Wiley and Sons, New York. 2000.
3. Douglass, Introduction to the spectroscopic methods for the identification organic compounds – II, Oxford publications, 2009.
4. William Kemp, Organic Spectroscopy, 3rdEdn.McMillan, 1991.
5. Y.R.Sharma, Elementary Organic Spectroscopy 3rd., S.Chand, 1999.
6. R.M. Silverstein, G.D. Bassler and Monsu, Spectrometric identification of Organic compounds, Sixth Edn. John Willey and Sons, New York, 2005.
7. Carington and Ad.Mclachlan, Introduction to Magnetic Resonance, Harper and Row, New York, 1967.
8. P.S.Kalsi, Spectroscopy of Organic Compounds, 4

Syllabus:

SEMESTEER-II

CH921A Inorganic Photochemistry & Materials Science

Course Code	**CH921A**	**Credit**	**4**
Instruction Hours per Week	**4**	**Marks**	**CIA (50) / SE (50)**
Course Objective	• To provide the students with basic information on matter radiation interactions and their consequences excited state formation modes, photophysical and photochemical deactivation pathways, and application of theoretical knowledge. • Students are equipped with the knowledge on composition, molecular and electronic structures of inorganic compounds. • Students will know to identify and quantify the course of photophysical and photochemical processes.		

Course outcomes

On successful completion of this Course, the students will be able to

S. No	Course outcomes Statement	Cognitive Level
CO-1	Understand the photochemical pathways in various chemical reactions	K1, K2
CO-2	Elucidate the photophysical kinetics of unimolecular reaction evaluating using Stern-Volmer equation.	K3, K4
CO-3	Understand weak and strong interaction in photochemical process and construct a mechanism for transformation of low energy reactants to high energy products.	K2, K5
CO-4	Elucidate the mechanism involved in various metal complex systems.	K4
CO-5	Learn and apply the principles of the materials and constructing a reaction methodology using various precursor molecules.	K3, K4, K6
CO-6	Elucidate the imperfections in the crystal lattice and describing the phase transformation in inorganic materials.	K4, K5

Mapping of CO with PO and PSO

CO	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)						
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	Mean Scores of Cos
CO1	3	3	3	3	2	3	3	2	3	2	2	2.64
CO2	3	3	3	3	2	3	3	3	3	3	2	2.82
CO3	2	3	3	3	2	3	3	3	3	2	2	2.64
CO4	3	3	3	3	2	3	3	3	3	2	2	2.73
CO5	3	2	3	3	2	3	3	3	2	3	2	2.64
CO6	3	3	3	3	2	3	3	3	3	2	2	2.73
Mean Overall Score												2.70
Result												High

Assessment Pattern

Bloom's Category	CA Tests (Marks Allotment)		Term End Exam (100) Marks Allotment
	I CA (50)	II CA (50)	
Remember	10	10	20
Understand	10	10	30
Apply	10	10	20
Analyze	10	10	10
Evaluate	5	5	10
Create	5	5	10

Course content:

Unit - I: Basics of Photochemistry **15 Hours**

Principle-Light Dual nature-Basic Laws of Photochemistry-Quantum Yield. Selection rule-Notation for excited state Organic Compounds-Energy level for Inorganic Complexes.Absorption Spectra-Emission Spectra-Frank Condon Principle-Energy Dissipation by radiative and non radiative transfers. Quantum yield measurement-Actinometers-types of actinometers.Excited states of metal complexes-Charge transfer spectra, metal–centered transitions, charge transfer excitations, emission spectra. Photophysical Kinetics of Unimolecular reaction. Stern-Volmerequation.

Unit - II: Photochemistry of Transition Metal Complexes and Its Applications

Electron transfer reactions in transition Metal Complexes-Photo physical and photochemical implications of transition metal complexes. Weak Interactions and Strong interactions(Excited state as redox Reactants-redox Properties of bpy and Phencomplexes (Fe, Ru and Os). Energy and electron transfer-Application of redox processes of electronically excited states for catalytic purposes. Transformation of low energy reactants into high energy products, chemical energy into light. Storage of light energy-EndoergonicProcess(Honda's cell)-Photo electrochemical cell

Unit – III: Photochemical Applications of Inorganic Systems
Metal complex sensitizer(Fe and Ru Systems) Metal Colloid systems, semiconductor supported metal or oxide systems (TiO_2 supported systems). Photoproduction of Hydrogen and Oxygen-Water photolysis. Spectra of Organometallics-Metal Carbonyl compounds, Organometallic compounds with metal-metal bonding. Photochemistry in the solid state.

Unit - IV: Preparative Techniques
Principles of solid-state synthesis- ceramic methods, solid solution and compound precursors (nitrates, carbonates, hydroxides, cyanides and organometallics), sol-gel, spray pyrolysis, combustion, hydrothermal, electrosynthetic techniques -
New Materials: Fullerenes and fullerides: structure, synthesis, functionalization approaches, conducting properties of fullerides-applications. NASICON and alumina–structure and conducting properties. High-Tc Oxides - structure, perovskite A & B, structure and synthesis of La, Sr and Ba cuprates-applications.

Unit V
Crystal imperfections, Diffusion in solids, phase transformations, elastic, inelastic and visco elastic behavior.
Point Imperfections, The Geometry of Dislocations, Other Properties of Dislocations, Surface Imperfections. Fick's Laws of Diffusion, Solution to Fick's Second Law, Applications Based on the Second Law Solution, The Kirkendall Effect, The Atomic Model of Diffusion, Other Diffusion Processes. Phase Transformations, Time Scale for Phase Changes, nucleation and growth, The Nucleation Kinetics, The Growth and the Overall Transformation Kinetics. Elastic Behaviour-Atomic Model of Elastic Behaviour, The Modulus as a Parameter in Design, Rubber-like Elasticity. Anelastic behaviour, Relaxation Processes. Viscoelastic behaviour, Spring-Dashpot Models.

References

1. Gerald B. Porter, J.Chem.Edu,1983, 60, 785.
2. K. K. Rohatgi-Mukerjee, Fundamentals of Photochemistry,New Age International Publishers, Calcutta.
3. Balzani, V.; Bolletta, F.; Scandola, F.; Ballardini. R.Pure and Appl. Chem.,1979, 51, 299.
4. John S. Connolly, Photochemical ConversionAnd Storage Of Solar Energy,Academic Press, New York,1981.
5. Balzani, V.; Cassarati, V.Photophysics and Photochemistry of coordination compounds, Academic Press, Newyork, 1970.
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7. S. Arunachalam, Inorganic photochemistry, Kala publications, Trichy, 2002.
8. D. M. Roundhill, Photochemistry and Photophysics of Metal complexes, Springer; Edition, 1994.
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11. M. G. Arora, Solid State Chemistry by Anmol Publications, New Delhi, 2001.
12. P. K. Palanisamy, Materials Science, Scitech Publications, Chennai, 2003
13. Geoffrey A Ozin and Andre C Arsenault, Nanochemistry, A chemical approach to Nanomaterials, RSC, 2006.
14. Harry R Allcock, Introduction to materials chemistry, Wiley NY, 2008
15. Gurtu and Gurtu, Solid state Chemistry, Pragathiprakashan, 2015.
16. V. Raghavan, material Science and Engineering, Eastern Economic Edition, New Delhi, 2011.
17. Dr. Elangoven, Solid State Physics

Syllabus

SEMESTER-II

CH921B – Polymer Chemistry

Course Code	**C327**	**Credit**	**4**
Instruction Hours per Week	**4**	**Marks**	**CIA (50) / SE (50)**
Course Objective	• To gain knowledge in the preparation, properties, characterization and uses of polymers. • To appreciate the role and applications of polymer substances.		

Course outcomes:

On successful completion of this Course, the students will be able to

S.No	Course outcome Statement	Cognitive Level
CO-1	Understand different types of polymers and learning the polymerization techniques	K1, K2
CO-2	Enumerate the reaction mechanism that takes place in the polymers	K3, K4
CO-3	Demonstrate the structural morphology of polymers	K2, K5
CO-4	Determining the molecular weights using different techniques.	K4
CO-5	Devise synthetic methodology for industrial polymers and assessing its importance	K4, K5
CO-6	Elucidate the synthetic methods of various novel polymers.	K4, K6

Mapping of CO with PO and PSO

CO	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)						
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	Mean Scores of Cos
CO1	3	3	3	3	2	3	3	2	2	2	1	2.45
CO2	3	3	3	3	2	3	3	2	2	2	2	2.54
CO3	3	2	3	3	2	3	3	2	2	3	3	2.6
CO4	2	3	3	2	2	3	3	2	2	2	2	2.36
CO5	3	3	3	3	2	3	3	2	2	3	2	2.63
CO6	3	3	3	3	2	3	3	2	2	3	2	2.63
Mean Overall Score												2.53
Result												High

Assessment Pattern

Bloom's Category	CA Tests (Marks Allotment)		Term End Exam (100) Marks Allotment
	I CA (50)	II CA (50)	
Remember	10	10	20
Understand	10	10	30
Apply	10	10	20
Analyze	10	10	10
Evaluate	5	5	10
Create	5	5	10

Course content:

Unit - I: Basic Concepts

Classification: natural, synthetic, organic, inorganic, elastomers, fibers, resins, and plastics: thermoplastic and thermosetting. -Nomenclature and isomerism-polymerization-functionality-Molecular forces and chemical bonding in polymers-Molecular Weight-Linear, branched, and cross-linked polymers. Techniques of polymerization–emulsion, bulk, solution and suspension.

Unit - II: Reaction, Mechanism and Kinetics

Reaction of polymers (Addition, Hydrogenation, Hydrolysis Cyclisation and Cross linking) Kinetics and Mechanism of polymerization-free radical, cationic, anionic and co-ordination polymerization (Ziegler-Natta Catalyst). Copolymerization-Kinetics (Detailed Study). General characterization–Kinetic chain length–degree of polymerization, chain transfer-initiators-inhibitors-retarders.

Unit - III: Structure, Properties, Polymer Characterization and Analysis

Structure –Physical Property-Morphology (configurations-crystal structure-morphology-crystallization and melting)-Rheology (Viscoelasticity-glassy state and glass transition) Factors affecting Glass transition temperature-crystallinity and melting point-related to structure. Crystalline nature determination-X-Ray diffraction- Thermo Gravimetric Analysis-molecular weight determination-Osmometry(membrane), Ultra centrifuge, and Gel Permeation Chromatography.

Unit - IV: Industrial and Natural Polymers

Important industrial polymers-preparation and application of polyethylene, polyvinylchloride, poly urethanes, polytetrafluro ethylene (TEFLON), Nafion and ion-exchange resins. Importance of natural polymers-application and structures of starch, cellulose, chitin and chitosan derivatives.

Unit - V: Novel Polymers

Polymers in Medicine-Ionomers-Electronically conducting polymers-Interpenetrating polymer networks-Inorganic Polymers-Polymer liquid Crystals-High temperature and fire-retardant polymers-polymer nanocomposites- Electroluminescent polymers.

References

1. F. W. Bill Meyer. Text book of polymer science, III Edition, John Wiley and sons, New York, 1973.
2. V. R. Gowarikar, B. Viswanathan, J. Sridhar, Polymer Science, Wiley Eastern, 1986.
3. G. S. Misra, Introduction to Polymer Chemistry, New Age Publishers Ltd. 2008,
4. C. E. H. Brawn, The Chemistry of High Polymers, Butter worth & Co., London, 1948.
5. G. Odian, Principles of Polymerization, McGraw Hill Book Company, New York, 1973.
6. E. A. Coolins, J. Bares and E. W. Billmeyer, Experiments in Polymer Science, Wiley Interscience, New York, 1973.
7. Jagdamba Singh, R. C. Dubey, Organic Polymer Chemistry, PragathiPrakashan, 3rd Edn., 2011.
8. Rudin, The Elements of Polymer Science and Engineering. Academic Press, New York, 1973.
9. G. S. Krishenbaum, Polymer Science Study Guide, Gordon Breach Science publishing, New York, 1973.

Online Source

1. https://hackr.io/tutorials/learn-polymer

Syllabus

SEMESTER-II

Chemoinformatics

Course Code	CH921C	Credit	4
Instruction Hours per Week	4	Marks	CIA (50) / SE (50)
Course Objective	• To study the fundamentals principles of the various computational methods • To interpret the various methods of representing molecules in a chemical database • To learn to analyse the data available in various databases • To learn to apply the datamining tools on datasets and interpret the results		

Course Outcomes

- On successful completion of this Course, the students will be able to

S. NO	Course Outcomes Statement	Cognitive level
CO1	Describe the various methods of representing molecules in a chemical database and apply the various tools.	K1 & K3
CO2	Analyze the physicochemical data available in various databases	K4
CO3	Apply the data mining tools on datasets and interpret the results.	K2 & K3
CO4	Explain the fundamentals and apply the various computational methods in chemical calculations.	K1 & K3
CO5	Evaluate the chemical calculations using computer programs, construct the new molecule using molecular modelling tools	K5 & K6
CO6	Design the structure of the small molecules and integrate the docking process using the software	K3 & K6

Mapping of CO with PO and PSO

CO	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)						
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	Mean Scores of Cos
CO1	3	3	3	3	2	3	3	3	3	3	2	2.81
CO2	3	3	3	3	2	3	3	3	3	3	2	2.81
CO3	3	3	3	3	2	3	3	3	3	3	2	2.81
CO4	3	3	3	2	2	3	3	3	3	3	2	2.72
CO5	3	3	3	3	2	3	3	3	2	3	2	2.72
CO6	3	3	2	3	2	3	3	3	2	3	3	2.72
Mean Overall Score												2.76
Result												High

Assessment Pattern

Bloom's Category	CA Tests (Marks Allotment)		Term End Exam (100) Marks Allotment
	I CA (50)	II CA (50)	
Remember	10	10	20
Understand	10	10	30
Apply	10	10	20
Analyze	10	10	10
Evaluate	5	5	10
Create	5	5	10

Course content

Unit – I: Introduction to Chemoinformatics

History and evolution of Chemoinformatics, Use of Chemoinformatics, Prospects of Chemoinformatics, Molecular modelling, and structure elucidation. Nomenclature: IUPAC names, trade names, common names., Representing the molecules: Older systems – Connection tables, Line notation – INCHI, SMILES, WLN canolications. (Activity – Create a SMILES notation of simple molecules using the software) Line notation versus connection tables. Query languages - SMARTS, SMILES coding, Matrix representations, Introduction to chemical structure file formats - Molfiles and Sdfiles

Unit – II: Structure Searching

Structure searching:2D-Fingerprints-Structural Keys – Hashed fingerprints, Exact structure searching, Substructure search, Sub structure searching - screening methods- algorithms for sub graph isomorphism – practical aspects of structure searching - Ways to measure Similarity - 2D topology, 3D configuration, Tanimotto Coefficient – Euclidean distance – Dice Coefficient – Cosine Coefficient – Tversky similarity Coefficient.Basics of computation of physical and chemical data and structure descriptors, data visualization

Unit – III: Databases and Datamining

Introduction-Database concepts-**types**-chemical, proteomic, genomic and literature databases-source, content and design, applications.
Chemical databases-Chembank, ChemPDB, Combichem, NCI- Pubchem (Compounds, Substances, Bioassay), PubMed, Drug Bank, ChemSpider (Activity - Search the simple molecules and predict their physico – chemical properties using Pubchem database)
Introduction-Aspects of Data mining – Techniques of Data mining – Multi dimensional models – cube – star – snowflakes – classification techniques – K-nearest neighbour – Decision tree –– Baeysian classifier – Introduction to neural network- Applications of Data mining

Unit IV: Molecular Modelling and Docking:

Molecular descriptors – ID, 2D & 3D – Deriving a simple QSAR equation – Hansch analysis – Free Wilson analysis – Application of Hansch equation – Hydrophobic & Steric factors – Influence of electronic factors – Ionisation constants, QSPR - Toxicity relationship

Ligand based drug design – Structure based drug design – Docking & Scoring functions – Active site characterization, building a molecule and energy optimization using ARGUSLAB (Activity),Docking of small molecules using ARGUSLAB (Activity)

Unit V: Computational chemistry
Fundamental principles - Ab initio methods – HartreeFock approximations – semi empirical methods – density functional theory – Basic theory – Linear scaling techniques – molecular mechanics - Basic theory – existing force fields – molecular dynamics and Monte Carlo simulations.

Reference Books:

1. Andrew R. Leach, Valerie J. Gillet. An Introduction to Chemoinformatics, revised edition, Springer, Netherland, 2007.
2. Larsen et al (ed), Textbook of Drug Design and Discovery, 3rd edition, Taylor and Francis, London and NewYork, 2004.

3. Leach A.R, Molecular Modelling: Principles and applications, 2nd edition, Prentice Hall, New Delhi, 2001.

4. K.V. Raman, Computer Applications in Chemistry, Tata McGraw Hill, New Delhi, 2008.

5. Vikas Gupta, Computer Course Kit, Dream Tech Press, 2010

Web sources:

1. https://open-babel.readthedocs.io/en/latest/Cheminf101/index.html

2. https://open-babel.readthedocs.io/en/latest/Cheminf101/represent.html#iupac-names-trade-names-common-names

3. https://open-babel.readthedocs.io/en/latest/Cheminf101/similarity.html

4. http://insideinformatics.cambridgesoft.com/webinars/info/Default.aspx?webinarID=632

5. http://www.acdlabs.com/resources/freeware/chemsketch/

6. http://www.acdlabs.com/download/technotes/2016/technote_chemsketch_advanced.pdf

7. accelrys.com/products/pdf/**isis-draw**.pdf

8. http://www.originlab.com/doc/Tutorial

9. http://www.inflibnet.ac.in/

10.https://www.**khanacademy**.org/

Syllabus:

SEMESTER-II

Organic Chemistry-IV

Course Code	**CH1017**	**Credit**	**4**
Instruction Hours per Week	**4**	**Marks**	**CIA (50) / SE (50)**
Course Objective	• To know modern synthetic methods and synthetic strategies. This help in planning the synthesis of any types of organic compounds. • To learn the synthesis and bio-synthesis of heterocyclic products.		

Learning Outcomes:

- Any types of organic compounds synthesis were learned by the students, through modern synthetic methods and strategies.
- Synthesis and bio-synthesis of heterocyclic products were also learned by the students

Course Outcomes:

Sl. No.	Course Outcome Statements	Knowledge level
	On successful completion of this Course, students will be able to	
CO1	Define the modern synthetic terminologies/methods and build the synthetic strategies incorporated in retrosynthesis of various types of organic molecules	**K1, K6**
CO2	Identify suitable protecting reagents for the protection of multifunctional organic molecules and predicting suitable deprotecting reagents after the completion of desired reaction.	**K1, K2**
CO3	Sketch various heterocyclic compounds structure with numbering and their interaction with various chemical reagents in detail.	**K3**
CO4	Illustrate the importance of environmentally benign solvents and their role in synthetic organic reactions.	**K4**
CO5	Validate the structure of various natural organic molecules and confirming their structure through total synthesis	**K5**
CO6	Build the synthetic route theoretically for a given target molecule in retrosynthetic way with theoretical justification.	**K6**

Mapping of CO with PO and PSO

CO	Programme Specific Outcomes (PSO)						Programme Outcomes (PO)					Mean Scores of COs
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PO1	PO2	PO3	PO4	PO5	
CO1	3	3	3	2	2	2	3	3	2	2	2	2.4545455
CO 2	3	3	2	2	2	2	3	2	2	2	2	2.2727273
CO 3	3	3	3	3	2	3	3	3	3	2	2	2.7272727
CO 4	3	2	3	3	3	3	3	2	3	3	1	2.6363636
CO 5	3	2	3	2	2	3	2	2	3	3	1	2.3636364
CO 6	3	3	3	3	2	2	3	3	3	3	1	2.6363636
Mean Overall Score												2.515152
Result												

Assessment Pattern

Bloom's Category	CA Tests (Marks Allotment)		Term End Exam (100) Marks Allotment
	I CA (50)	II CA (50)	
Remember	10	10	20
Understand	10	10	30
Apply	10	10	20
Analyze	10	10	10
Evaluate	5	5	10
Create	5	5	10

Course Content

Unit - I: Retrosynthetic Analysis-I **12 Hours**

Basic guidelines and terminology of retrosynthesis (synthons, FGI, disconnection approach), Important functional group interconversion synthesis of aromatic compounds-, one group C-X disconnections and two group C-X disconnections, one group C-C disconnections and two group C-C disconnections, important strategies of retrosynthesis.

Unit - II: Retrosynthetic Analysis-II and Protecting Functional Groups **12 Hours**

Amine and alkene synthesis, umpolung carbonyl group reactivity in synthesis, Protection and deprotection of hydroxy, carbonyl, amine and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection; illustration of protection and deprotection in synthesis.

Unit - III: Chemistry of heterocyclic compounds **12 Hours**

Numbering of heterocyclic compounds, structure, preparation and reactions of heterocyclic compounds (pyrrole, furan, thiophene, 1,2- and 1,3-azoles, triazoles, pyridine, pyryliums, diazines, triazine), Fused heterocycles containing one or more heteroatoms (indoles, benzofurans, benzothiophene, benzenellated azoles, quinolines, isoquinolines, benzopyrones).

Unit - IV: Green chemistry and Natural Products Chemistry **12 Hours**

Green chemistry: Importance and synthetic reactions of green solvents as reaction medium (water, $ScCO_2$, Polyethylene glycol)- Ionic liquids (alkylation and coupling reactions)-microwave assisted organic synthesis.

Steroids: Sterols and bile acids, estrogens, androgens: **Alkaloids:** Structure, synthesis Reserpine, Morphine.**Terpenoids:**Zingiberene, Squalene. Natural Pigments: structural confirmations of flavones, flavanones, isoflavones, xanthones, quinones.

Unit - V: Bioorganic Molecules **12 Hours**

Molecular structure and numbering of Purines (Uric acid, Cytosine, Adenine, Guanine) &Pyrimidines (Uracil, thymine & Cytosine). Nucleic acids-Functions of nucleic acids- Structural features of nucleosides and nucleosides-structure and biological implications of DNA and RNA (m-RNA, t-RNA and r-RNA) - replication of DNA - Genetic code and informational theory. Proteins – standard amino acids - peptide synthesis-End group analysis (Sanger's method, Edmon's degradation) - primary, secondary, tertiary structure and quaternary structure of proteins and their determination.

References

1. William Caruthers and Iain coldham, Modern methods of organic synthesis, IV Edition, Cambridge university press, 2004.
2. Michael B Smith, Organic Synthesis, Tata Mc Graw Hill, 1994.
3. Stuart warren, Organic synthesis the disconnection approach,Wiley India edition, 2004.
4. V K Ahluwalia and Renuagarwal Organic synthesis special techniques, second edition, Narosa Publishing House, 2007.
5. J.March, Advanced Organic Chemistry, 4thEdn, Wiley Publications, 1992.
6. Gurdeep R Chatwal, Organic Chemistry of Natural Products, Vol 1 & 2, revised Edn., Himalaya Publications, 2009.
7. O.P Agarwal, Chemistry of Organic Natural Products, Vol 1 & 2, Goel Publications, 28thEdn., 2002.
8. S.P.Bhutani, Chemistry of Biomolecules, Ane Books, 2009.
9. George S. Zweifet, Michael H Nantz, Modern Organic Synthesis – an introduction, W.H.Freeman and Company, 2007.
10. Raj K Bansal, Heterocyclic chemistry, fourth edition, New Age International Publishers, 2005.

Syllabus:

SEMESTER-II

Inorganic Chemistry-IV

Course Code	**CH1018**	**Credit**	**4**
Instruction Hours per Week	**4**	**Marks**	**CIA (50) / SE (50)**
Course Objective	• To illustrate the structure and bonding nature of Organometallic compounds and their reactions. • To study the various industrial importance and applications of organometallic compounds. • To study the fundamentals of nuclear chemistry and learn about the working principle of nuclear reactor. • To learn the MO theory and spectral behaviour in coordination compounds. • To learn the structure and function of bio – inorganic compounds. • To study the application of metals in medical field.		

Course Outcomes

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

S. NO	Course Outcomes Statement	Cognitive level
CO1	Students can explain the bonding in organometallic compounds and illustrate the different types of reactions of complexes	**K1, K2 & K3**
CO2	Students can analyse the catalytic properties of organometallic compounds and to integrate the application of these compounds in catalysis.	**K4 & K6**
CO3	Students will be able to discuss the aspects of nuclear chemistry and applications of nuclear fission and fusion reactions	**K2 & K3**
CO4	Students can understand and apply the MO theory and construct the Orgel and Sugano - Tanabe diagrams for coordination complexes	**K1, K3 & K6**
CO5	Students can analyse the electronic spectra of complexes and can able to evaluate the Δ_0 and β	**K4 & K5**
CO6	Students can review the importance of metallo biochemistry and conclude the role of metals in medicine	**K4 & K5**

Mapping of CO with PO and PSO

CO	Programme Specific Outcomes (PSO)						Programme Outcomes (PO)					Mean Scores of COs
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PO1	PO2	PO3	PO4	PO5	
1	3	3	3	3	2	2	3	3	3	2	3	2.7
2	3	3	3	3	3	3	3	3	3	3	2	2.9
3	3	3	3	3	2	2	3	3	3	2	3	2.7
4	3	3	3	3	2	2	3	3	3	2	3	2.7
5	3	3	3	3	3	2	3	3	3	2	3	2.8
6	3	3	3	3	3	3	3	3	3	3	2	2.9
Mean Overall Score												2.8
Result												**High**

Assessment Pattern

Bloom's Category	CA Tests (Marks Allotment)		Term End Exam (100) Marks Allotment
	I CA (50)	II CA (50)	
Remember	10	10	20
Understand	10	10	30
Apply	10	10	20
Analyze	10	10	10
Evaluate	5	5	10
Create	5	5	10

Course Content

Unit - I: Organometallic Chemistry – I **12 Hours**

Carbon donors: Alkyls and aryls metalation, bonding in carbonyls and nitrosyls, chain and cyclic donors, olefins, acetylene and allyl system synthesis structure and bonding Metallocenes. Reactions: Association substitution, addition and elimination ligand promotion, electrophilic and nucleophilic attack on ligands. Carbonylation.Decorboxylation, oxidative addition and fluxionality.

Unit - II: Organometallic Chemistry – II **12 Hours**

Catalysis: Hydrogenation of olefins (Wilkinson's catalyst), hydroformylation of olefins using cobalt or rhodium catalysts (oxo process), oxidation of olefins to aldehydes and ketones (Wacker process) polymerization (Zeigler – Natta Catalyst); cyclooligomerisation of acetylene using nickel catalyst (Repee's catalyst); polymer-bound catalysts.

Unit - III: Nuclear Chemistry – I **12 Hours**

Nuclear Reactions: Types, reactions, cross section, Q-value, threshold energy, compound nucleus theory: high energy nuclear reactions, nuclear fission and fusion reactions as energy sources - comparison between nuclear fission and fusion - Liquid drop and the shell models of the nucleus. photonuclear and thermo nuclear reactions.

Stellar energy: synthesis of elements, hydrogen burning, carbon burning. Nuclear Reactors: fast breeder reactors, particle accelerators, linear accelerators, cyclotron and synchrotron. Radiation chemistry - interaction of radiation with matter - linear energy transfer (LET) - Bethe's equation - Chernkov radiation - absorption coefficient - linear and mass absorption coefficient.

Unit - IV: Coordination Chemistry **12 Hours**

Molecular orbital theory and energy level diagrams, Evidence for metal-ligand orbital overlap, Jahn-Teller distortion, charge - transfer spectra.

Term states for "d" - ions, energy diagrams, concept of weak and strong field ligands d-d transitions, Orgel and Sugano - Tanabe diagrams, spin orbit coupling, nephelauxetic effect, spectral and magnetic characteristics of transition metal complexes.

Unit - V: Bio-Inorganic Chemistry – II **12 Hours**

Characterization of O_2 bound species by Raman and infrared spectroscopic methods; representative synthetic models of heme and non-heme systems.Electron transfer proteins - active site structure and functions of ferredoxin, rubridoxin and cytochromes, and their comparisons.Vitamin B_{12} and cytochrome P_{450} and their mechanisms of action.Metals in medicine - therapeutic applications of cis-platin, radio-isotopes (e.g., Tc& I_2) and MRI agents.

Text Books

References

1. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, John Wiley and Sons 5th Edition, 1988.
2. K.F. Purcel and J.C. Kotz, Inorganic Chemistry, W.Saunders Co., 1977.
3. EAV. Epsworth, D.W.H. Rankin and S. Cradock, Structural methods in Inorganic Chemistry, Blackwell Scientific Publ. 1987.
4. G. Coates M.I. Green and K. Wade. Principles of Organo metallic chemistry, Methven Co., London 1988.
5. R.B. Jordon, Reaction mechanism of Inorganic and Organo metallic system, OUP, 1991.
6. P. Powell, Principles of Organo metallic chemistry, Chappmanan Han. 1998.
7. R.C. Mehrothra, A. Singh, Organo Metallic Chemistry, Wiley Eastern Co., 1992.
8. R.B. Heslop and K. Jones, Inorganic Chemistry, Elsevier Scientific Publ. 1976.
9. H.A. O Hill and P. Day, Practical methods in advanced inorganic chemistry, John Wiley, 1968.
10. G. Frielander, J.w. Kennedy and J.M. Miller, Nuclear and Radiochemistry, John Wiley and Sons, 1981.
11. HariJeevanArnikar , Essentials of Nuclear Chemistry, New Age International (P) Ltd., 2005.
12. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Univ. Science Books, 1994.
13. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life (An introduction and Guide), John Wiley & Sons, 1994.

Online Resources

1. http://nptel.ac.in/courses/104101079/
2. http://eacharya.inflibnet.ac.in/ Inorganic Chemistry (I/II/III)

Syllabus

SEMESTER-II

PHYSICAL CHEMISTRY III

Course Code	**CH1019**	**Credit**	**4**
Instruction Hours per Week	**4**	**Marks**	**CIA (50) / SE (50)**
Course Objective	• To study the importance and theory of ionic conductance. • To learn the concepts of electrode - electrolytic interface and structure of the double layer. • To learn the mechanism of electrode reactions and electron transfer process. • To illustrate the importance and industrial applications of different types of fuel cells. • To understand the concepts of various methods of energy calculation in many electron systems. • To apply the VB, MO and HMO theory to simple many electrons system.		

Course Outcomes

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

CO. No.	**Course Outcome Statement**	**Cognitive Level**
CO 1	Comprehend the concept of activity coefficient and ionic strength of electrolytes and to evaluate and relate the mean ionic activity coefficient of electrolytes.	**K3 &K5**
CO 2	Describe the structure of the electrified interface, and define and describe mathematically the capacitance of various model of double layer	**K1 & K2**
CO 3	Calculate and analyse the electron transport and kinetic overpotential for electrodes at which a one-step and multi-step electron reaction takes place.	**K3 & K4**
CO 4	Know about the behaviour of ions in solution phase under different conditions and its application towards different energy storage devices	**K1 & K3**
CO 5	Describe many-electron atoms with the various approximation methods and evaluate the energy and construct wave function of many electron atoms with suitable methods	**K2, K5 & K6**
CO 6	Describe the chemical bonding quantum mechanically with VB, MO and HMO theory and able to calculate the pi electron energy to simple systems.	**K2 & K3**

Mapping of CO with PO and PSO

CO	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)						
	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PSO1**	**PSO2**	**PSO3**	**PSO4**	**PSO5**	**PSO6**	**Mean Scores of COs**
CO1	3	3	3	2	2	3	3	3	3	3	2	2.7
CO2	3	2	3	3	2	3	3	2	3	3	2	2.6
CO3	3	3	2	2	2	3	3	3	3	2	3	2.7
CO4	3	3	3	2	3	3	3	3	3	3	3	2.9
CO5	3	3	2	3	2	2	3	3	3	3	2	2.5
CO6	3	2	3	3	2	3	3	3	3	3	3	2.7
Mean Overall Score												2.6
Result												High

Assessment Pattern

Bloom's Category	CA Tests (Marks Allotment)		Term End Exam (100) Marks Allotment
	I CA (50)	II CA (50)	
Remember	10	10	20
Understand	10	10	30
Apply	10	10	20
Analyze	10	10	10
Evaluate	5	5	10
Create	5	5	10

Course Content

Unit - I: Electro Chemistry – I

The nature of electrolytes –ion-ion and ion-solvent interactions. The Debye- Huckel theory of ion -ion interaction. Mean ionic activity and mean ionic activity coefficient - activity coefficient of strong electrolytes - determination of activity coefficient by electrochemical method.

Debye Huckel limiting law derivation and verification - limitation of Debye Huckel limiting law at appreciable concentrations of electrolytes - Debye - Huckel – Onsager equation derivation and validity. Conductivity at high frequency (Debye-Falkenhagen effect) and at high field strength (Wien effect).

Unit - II: Electro Chemistry – II

Electrode - electrolyte interface - adsorption at electrified interface - electrical double layer - electro capillary phenomenon - Lippmann equation - Structure of double layers - Helmholtz - Perrin, Guoy - Chapman and Stern model of electrical double layers.
Mechanism of electrode reactions - polarization and over-potential - the Butler-Volmer equation for one step and multistep electron transfer reactions - significance of electron exchange current density and symmetry factors - transfer coefficient and its significance.

Unit - III: Electro Chemistry – III

Mechanism of the hydrogen and oxygen evolution reactions. Diffusion - Fick's law of diffusion - Effect of ionic association on conductance- Electro-kinetic phenomena – Electro-osmosis. Streaming potential – electrophoresis.

Corrosion and passivation of metals - Pourbaix diagram - Evan's diagram - Modern Batteries – Nickel-metal hydride batteries, lithium secondary batteries. Fuel cells – History – Types of fuel cells – H_2 / O_2 fuel cells – Direct methanol fuel cells– Alkaline fuel cells – phosphoric acid fuel cells - Molten carbonate fuel cells (High temperature fuel cell) – Proton exchange membrane fuel cells (PEM Cells). electrodeposition - principle and applications.

Unit - IV: Applications of Quantum Chemistry – III

Approximation methods - Need for approximation – Perturbation Theory – Time independent Perturbation (First order only) - Application of Perturbation theory to particle in one dimensional box, anharmonic oscillator and helium atom – Variation method – principle – methodology and its applications to hydrogen and helium atoms. Semi - empirical methods - Slater orbital and HFSCF methods.

Unit - V: Applications of Quantum Chemistry – IV

The Born - Oppenheimer approximation – VB and MO theories as applied to hydrogen molecular ion (H_2^+) and hydrogen molecule – coulomb integral an exchange integral and an overlap integral. Construction of sp, sp2 and sp3 hybrid orbitals - Huckel molecular orbital theory – principles and applications to ethylene, butadiene and benzene. Huckel calculation of pi- electron energies.

TEXT BOOKS

1. J.O.M. Bokris and A. K. N. Reddy, Electrochemistry, Vol. 1, 2A and 2B, Plenum, New York, 1977
2. Donald A McQuarrie, Quantum chemistry, Indian Edition, Viva Books Private Limited 2005.

REFERENCES

1. S. Glasstone, Introduction to Electrochemistry, Affiliated East West Press, New Delhi 1960.
2. D.R.Crow, Principles and Applications to Electrochemistry, Chapman and Hall 1991
3. ViswanathanB.,M.AuliceScibioh, Fuel Cells-Principles and Applications, Universities Press, Hyderabad, India, 2006
4. J. Robbins, Ions in Solution - An Introduction of Electrochemistry, Clarendon Press, Oxford, 1972
5. B.K.Sharma, Electrochemistry, Krishna Education publication, 2019.
6. R.K. Prasad, Quantum Chemistry, 1st Edition, New Delhi, Wiley Eastern Ltd, 1992.
7. Anderson J. M. Mathematics of Quantum Chemistry, I Edition, Massachusetts, A.Benjamine Inc.,1966

Online resource:

1. http://eacharya.inflibnet.ac.in/ Physical Chemistry-I (Quantum Chemistry) [32 lectures]

Syllabus

SEMESTER-II

Organic Chemistry Practical – II

Course Code	**PCH1013**	**Credit**	**4**
Instruction Hours per Week	**4**	**Marks**	**CIA (50) / SE (50)**
Course Objective	• To learn practical skills about the estimation of some organic compounds using chemical procedures		

Course Outcomes:

Sl. No.	**Course Outcome Statements**	**Knowledge level**
	On successful completion of this Course, students will be able to	
CO1	Analyze the unknown concentration of the given substance	K3
CO2	Synthesis and prepare simple organic compounds using a two stage process	K3, K6
CO3	Relate and articulate the fundamental principles of volumetric estimations	K5
CO4	Examine and evaluate data collected to determine the identity, purity, and yield of products	K5
CO5	Develop methods for the estimation of organic substances volumetrically	K6
CO6	Investigate and interpret simple organic compounds using IR, UV, Mass and NMR spectroscopic data	K2

Mapping of CO with PO and PSO

CO	Programme Specific Outcomes (PSO)						Programme Outcomes (PO)					Mean Scores of COs
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PO1	PO2	PO3	PO4	PO5	
CO1	3	2	3	3	3	1	3	3	2	3	1	2.4545455
CO 2	3	2	2	3	2	2	3	2	3	3	2	2.4545455
CO 3	3	3	3	3	2	1	3	3	2	3	2	2.5454545
CO 4	3	3	3	3	3	1	3	2	2	3	2	2.5454545
CO 5	3	2	2	3	3	1	3	2	2	2	2	2.2727273
CO 6	3	2	3	3	2	1	3	2	2	2	3	2.3636364
											Mean Overall Score	2.439394
											Result	

Course Content

Estimations

- Estimation of phenol
- Estimation of Aniline
- Estimation of Ketone
- Estimation of Glucose
- Saponification value of oil
- Iodination value of oil

Preparations (double stage)

- Sym. tribromo benzene from Aniline
- Benzanilide from benzophenone
- m-nitro benzoic acid from methyl benzoate
- 2,4- dinitro phenyl hydrazine from p-nitro chlorobenzene

SPECIAL INTERPRETATION OF ORGANIC COMPOUNDS UV, IR, PMR AND MASS SPECTRA OF THE FOLLOWING 15 COMPOUNDS (**any 10 may be chosen**)

- 1,3,5- Trimethyl benzene
- Pinacolane
- n-Propylamine
- p-Methoxy benzyl alcohol
- Benzyl bromide
- Phenylacetone
- 2-Methoxyethyl acetate
- Acetone
- Isoopropyl alcohol
- Acetaldehyde diacetate
- 2-N,N-Dimethylamino ethanol
- Pyridine
- 4-Picoline
- 1,3-dibromo - 1, 1- dichloropropene
- Cinnamaldehyde

References

1. N.S. Gnanapragasam and B. Ramamoorthy, "Organic Chemistry Lab Manual", S. Visvanathan Printers & Publishers,2006.
2. Arthur I. Vogel, "A Textbook of Practical Organic Chemistry", ELBS, 1985.

3. Scheme of Valuation

4. External Component: 50 Marks

S. No	Components	Mark Distribution
1	Estimation	20
2	Preparation	15
3	Interpretation of Spectra	05
4	Viva-Voce	05
5.	Record	05
	Total Marks	**50 Marks**

5.

6. <u>Mark distribution for components one and two in External</u>

7. i) Estimation error percentage for estimation

8. <2% - 20 marks

9. 2-3% - 20-15 marks

10. 3-4% - 15-10 marks

11. >4% - 05 marks

12. ii) Two stage preparation:

13. Stage -1 crude = 06 Marks

14. Stage -2 crude = 06 Marks

15. Re-crystallization = 03 Marks

16. Internal Component: 50 Marks

S. No	Components	Mark Distribution
1	Estimation	15
2	Two stage Preparation	15
3	Viva-voce	05
4	Theory of Practicals	05
5	Model practical examination	10
	Total Marks	**50 Marks**

17.

18. Conditions for Internal Component:

19. For Component **1** & **2,** 60% of the work done has to be taken in account

20. One Viva and one TOP per semester has to be conducted and taken into account

21.

22. <u>Mark distribution for components one and two in Internal</u>

23. i) Estimation error percentage for estimation

24. <2% - 15 marks

25. 2-3% - 15-10 marks

26. 3-4% - 10-05 marks

27. >4% - 05 marks

28. ii) Two stage preparation:

29. Stage -1 crude = 06 Marks

30. Stage -2 crude = 06 Marks

31. Re-crystallization = 03 Marks

SEMESTER-II

PCH1014 - Inorganic Chemistry Practicals – II

Course Code	**C327**	**Credit**	**4**
Instruction Hours per Week	**4**	**Marks**	**CIA (50) / SE (50)**
Course Objective	• To learn the methods and techniques to estimate inorganic metals.		

Course Outcomes

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

S. NO	Course Outcomes Statement	Cognitive level
CO1	Gain knowledge about the methods and techniques to estimate inorganic metals	**K1, K2**
CO2	Analyse the complex materials, alloys or ores and ions	**K5**
CO3	Detecting the amount of mixtures of iron -magnesium, iron – nickel, copper - nickel and copper – zinc by Gravimetric and Volumetric	**K4**
CO4	Understand Photoelectric method	**K2**
CO5	Solve the spectra and interpreting it	**K2, K6**

Mapping of CO with PO and PSO

CO	Programme Specific Outcomes (PSO)						Programme Outcomes (PO)					Mean Scores of COs
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PO1	PO2	PO3	PO4	PO5	
1	3	2	3	2	3	3	3	2	3	3	1	2.5
2	3	2	2	3	3	3	3	3	3	3	1	2.6
3	3	2	2	2	3	3	3	2	2	3	1	2.4
4	3	2	3	3	3	2	3	3	3	3	1	2.6
5	3	3	2	2	3	2	3	3	2	3	1	2.5
6	3	2	3	2	3	3	3	2	3	3	1	2.5
Mean Overall Score												2.5
Result												**High**

Course Content

Semimicro qualitative analysis of mixture containing two common and two rare cations.

The following are the rare cations to be included. W, Ti, Te, Se, Ce, Th, Zr, V, U, Li, Mo, Be.

Complexometric Titrations (EDTA) - Estimation of Ca, Mg and Zn.

- Preparation of the followings:
- Potassium tris (oxalate) aluminate (III) trihydrate
- Tris (thiourea) copper (I) chloride
- Potassium tris (oxalaato) chromate (III) trihydrate
- Sodium bis(thiosulphato) cuprate (I)
- Tris (thiourea) copper (I) sulphate
- Sodium hexanitrocobaltate (III)
- Chloropentammine cobalt (III) chloride
- Bis (acetylacetonato) copper (II)
- Hexamminenickel (II) chloride
- Bis (thiocyanato) pyridine manganese (II)

Text Books

1. V. V. Ramanujam, Inorganic Semimicro Qualitative Analysis; 3rd ed., The National Publishing Company, Chennai, 1974.

2. Vogel's Text book of Inorganic Qualitative Analysis, 4 th Ed, ELBS, London, 1974.

Scheme of Valuation

External Component:

Components	**Marks**
Volumetric and Gravimetric	20+20
Colorimetric analysis	20
Spectral interpretation & short procedure	10+10
Viva	10
Record	10
Total	**100 Marks**

Total Marks 100 is converted in to 50 marks

Internal Component:

Components	Marks
Volumetric and Gravimetric	10+10
Colorimetric analysis	10
Model exam	10
Theory of practical	05
Viva	05
Total	**50 Marks**

Error Analysis

Volumetric analysis

< 2 - 20 marks

2-3 - 20 - 10 marks

3-4 -10 - 05 marks

>4 - 05 marks

Gravimetric analysis

< 2 - 20 marks

2-3 - 20 - 10 marks

3-4 -10 - 05 marks

>4 - 05 marks

Colorimetric Analysis

< 2 - 20 marks

2-3 - 20 - 10 marks

3-4 -10 - 05 marks

>4 - 05 marks

Syllabus

SEMESTER-II

PHYSICAL CHEMISTRY PRACTICALS II

Course Code	**PCH1015**	**Credit**	**4**
Instruction Hours per Week	**4**	**Marks**	**CIA (50) / SE (50)**
Course Objective	• To understand the principles that govern the basic electrochemical experiments • To learn the physical methods used in determination of parameters such as pH, conductance and EMF etc. •		

Course Outcomes

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

CO. No.	**Course Outcome Statement**	**Cognitive Level**
CO 1	**Define** the principle of conductometric and potentiometric titration.	K1
CO 2	**Explain** the conductometric titration of strong acid, weak acid and mixture of acids with strong Base.	K2
CO 3	**Determine** the equivalent conductance of strong electrolytes at infinite dilution and dissociation constant of weak electrolyte	K3
CO 4	**Calculate** the pH of a buffer solution using emf measurements	K4
CO 5	**Prepare** a salt bridge for potentiometric experiments.	K5
CO 6	Verify the various laws like Ostwald's dilution law and Kohlrausch's law conductometrically and design working electrodes	K6

Mapping of CO with PO and PSO

CO	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)						
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	Mean Scores of COs
CO1	3	3	2	2	2	3	2	3	3	2	1	2.36
CO2	3	3	2	2	2	3	2	3	3	2	1	2.36
CO3	3	3	3	2	2	3	3	3	3	2	1	2.55
CO4	3	3	3	3	2	3	2	3	3	3	1	2.64
CO5	3	3	3	3	2	3	2	3	3	3	1	2.64
CO6	3	3	3	3	3	3	2	3	3	3	1	2.73
Mean Overall Score												2.55
Result												High

Course Content

Conductivity Measurements

1. Determination of equivalent conductance of a strong electrolyte and verification of Debye - Huckel - Onsager Equation
2. Verification of Debye-Huckel limiting law
3. Verification of Ostwald's Dilution law for a weak electrolyte. Determination of PK values of weak acids and weak bases.
4. Conductometric titrations between acid (simple and mixture of strong and weak acids) - base, precipitation titrations including mixture of halides.

E.M.F Measurements

5. Determination of standard potentials (Copper & Zinc)
6. Determination of thermodynamic quantities from EMF measurements - potentiometric titrations.
7. Determination of pH and calculation of pKa.
8. Determination of stability constant of a complex.
9. Determination of solubility product of a sparingly soluble salt. Redox titrations.
10. Precipitation titration of mixture of halides by EMF measurements.

Spectroscopy

11. Experiments given only to familiarize the interpretation of spectra provided. Interpretation of simple UV-Visible spectra of simple molecules for the calculation of molecular data and identification of functional groups (5 typical spectra will be provided).
12. IR and NMR spectral calculations of force constant - identification and interpretation of a Compound.

List of Experiments Suggested for Physical Chemistry Practical - II

Typical list of possible experiments is given. Experiments of similar nature and other experiments may also be given. The list given is only a guideline. Any 15 experiments have to be performed in a year.

1. Determination of the equivalent conductance of a weak acid at different concentrations and verify Ostwald's dilution law and calculate the dissociation constant of the acid.
2. Determination of equivalent conductance of a strong electrolyte at different concentrations and examine the validity of the Onsager 's theory as limiting law at high dilutions.
3. Determination of the activity co-efficient of Zinc ions in the solution of 0.002M Zinc sulphate using Debye-Huckel limiting law.
4. Determination of the solubility product of silver bromate and calculate its solubility in water and in 0.01 M $KBrO_3$ using Debye-Huckel limiting law.
5. Conductometric titrations of a mixture of HCl, CH_3COOH and NaOH.
6. Determination of the dissociation constant of an acid at different dilution.
7. Determination of the solubility of the lead iodide in water, 0.04 M KI and 0.04 M Pb $(NO_3)_2$ at 298 K
8. Determination of the solubility product of lead iodide at 298 K and 308 K and calculate the molar heat of solution of lead iodide.
9. Compare the relative strength of acetic acid and mono chloroacetic acid by conductance method.
10. Determine the basicity of organic acids (oxalic /benzoic).
11. Determine the electrode potentials of Zn and Ag electrodes in 0.1M and 0.001M solutions at 298 K and fine the standard potentials for these electrodes and test the validity of Nernst equation.
12. Determine the activity co-efficient of an electrolyte at different molalities by EMF measurements.
13. Determine the dissociation constant of acetic acid titrating it with sodium hydroxide using quinhydrone as an indicator electrode and calomel as a reference electrode.
14. Study of the electrolytic separation of metals (Ag, Cu, Cd and Zn)
15. Determine the strength of a given solution of KCl using differential potentiometric titration technique.
16. Determine the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.
17. Determine the transport number of Ag ions and nitrate ions by Hittorf's method.
18. Determine the transport number of cadmium ions and sulphate ions by measuring emf of concentration cells with and without transference.
19. Determine the dissociation constant of monobasic or dibasic acid by all the Alber-Serjeant method.
20. Determine the pH of the given solution with the help of indicators using buffer solutions and by colorimetric method.
21. Perform acid-base titration in a non-aqueous medium.
22. Determine the pH of a given solution by EMF method using glass and calomel electrodes and evaluate pKa value of an acid.
23. Determine the pH of a given solution by emf methods using hydrogen electrode and quinhydrone electrode.
24. Estimate the concentration of cadmium and lead ions by successive reduction in polarography.
25. Verify Illkovic equation.
26. Determine lead ion by amperometric titrations with potassium dichromate.
27. Determine ferric ion by amperometric titration.
28. Determine pH value of an acid-base indicator (methyl red) by colorimetry.
29. Determine the composition and instability constant of a complex by mole ratio method.
30. By colorimetry, determine simultaneously Mn and Cr in solution.
31. Study the effect of solvent on the conductivity of $AgNO_3$/acetic acid and determine the degree of dissociation and equilibrium constant in different degree of dissociation and mixtures (DMSO, DMF, dioxane, acetone, water) and test the validity of Debye-Huckel Onsager's equation.
32. Determine the solubility of $Ca(TiO_3)_2$ in deionized water and in dilute solution of KCl at 298 K. Determine the solubility product graphically.
33. Determine the equivalent conductivity of a Ca electrolyte and dissociation constant of the electrolyte.
34. Determine the equivalent dissociation constant of a polybasic acid.
35. Calculate the thermodynamic parameters for the reaction Zn + H_2SO_4 -------ZnSO4 + H2 by EMF method.

36. Determine the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.
37. Determine the stability constant of a complex by polarographic method.
38. Determine the g value from a given ESR spectrum.

Text books

1. B. Viswanathan and P.S. Raghavan, Practical Physical Chemistry, Viva Books, New Delhi,2009.
2. K. Sundaram, Practical Chemistry, S. Viswanathan Co. Pvt., 1996.

3.

4. Scheme of Valuation

5. External Component (50 Marks):

Name of the component	**Marks**
Spectral Interpretation	10
Experiment	30
Record	05
Viva – Voce	05
Total	**50**

6.

7. Internal Component (50 Marks):

Name of the component	**Marks**
Regular practical (Average of best 70%)	30
Theroy of practical (2)	05
Viva – Voce (2)	05
Model exam	10
Total	**50**

8.

9.

10. Marks distribution for Experiment / Regular Practical – 30 marks

Name of the component	**Marks**
Short procedure, formula and model graph	05
Calculation and graph	05
Result & accuracy	20
Total	**30**

11. Marks for results & accuracy for all experiments:

Error	**Marks**
≤5%	20
5.1-10%	20-10
>10%	5

12.

13.

14. Mark distribution PG – 2021 onwards

15. CA Components (PG)

Component	**Marks**
I CA	15
II CA	15
MCQ	10
Assignment/Seminar/Quiz Snap Test / problem solving/ Notes preparation / Journal paper reference (minimum any two)	10
Total	**50**