# SACRED HEART COLLEGE (AUTONOMOUS)

Tirupattur - 635 601, Tamil Nadu, S.India

Resi: (04179) 220103College: (04179) 220553Fax: (04179) 226423

A Don Bosco Institution of Higher Education, Founded in 1951 \* Affiliated to Thiruvalluvar University, Vellore \* Autonomous since 1987 Accredited by NAAC (4<sup>th</sup> Cycle – under RAF) with CGPA of 3.31 / 4 at 'A+' Grade

# M.Sc. Chemistry (CBCS)

Sem	Sub	Title of the paper	Ins	Cr	CA	Sem	Total
			Hrs		Mks	Mks	
	Core	Organic Chemistry – I	<mark>4</mark>	<mark>4</mark>	<mark>50</mark>	<mark>50</mark>	<u>100</u>
	Core	Inorganic Chemistry – I	<mark>4</mark>	<mark>4</mark>	<mark>50</mark>	<mark>50</mark>	<u>100</u>
	Core	Physical Chemistry – I	<mark>5</mark>	<mark>4</mark>	<mark>50</mark>	<mark>50</mark>	<u>100</u>
		Organic Practicals – I	<mark>4</mark>	<mark>-</mark>			
Ι	Core Practicals	Inorganic Practicals – I	<mark>4</mark>				
		Physical Practicals – I	<mark>4</mark>	-	-	-	_
		1. Analytical Chemistry					
		2. Green Chemistry	_	_			
	Elective - I	3. Pharmaceutical	<mark>5</mark>	<mark>5</mark>	<mark>50</mark>	<mark>50</mark>	<mark>100</mark>
		Chemistry					
	Core	Organic Chemistry – II	<mark>4</mark>	<mark>4</mark>	<mark>50</mark>	<mark>50</mark>	<mark>100</mark>
	Core	Inorganic Chemistry – II	<mark>4</mark>	<mark>4</mark>	<mark>50</mark>	<mark>50</mark>	<mark>100</mark>
	Core	Physical Chemistry – II	<mark>5</mark>	<mark>4</mark>	<mark>50</mark>	<mark>50</mark>	<mark>100</mark>
		1. Research Methodology					
		2. Heterocyclic Chemistry	~	-	50	70	100
	Elective - II	3. Bio-organic Chemistry	<mark>.</mark>	<mark>5</mark>	<mark>50</mark>	<mark>50</mark>	<mark>100</mark>
11							
	SSP	Reagents in Organic Chemistry	0	$2^*$			
		Organic Practicals – I	<mark>4</mark>	<mark>4</mark>	<mark>50</mark>	<mark>50</mark>	<mark>100</mark>
	Core Practicals	Inorganic Practicals – I	<mark>4</mark>	<mark>4</mark>	<mark>50</mark>	<mark>50</mark>	<mark>100</mark>
		Physical Practicals – I	<mark>4</mark>	<mark>4</mark>	<mark>50</mark>	<mark>50</mark>	<mark>100</mark>
	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
		1. Inorganic					
ш		photochemistry and					
	Elective - III	materials science	5	5	50	50	100
		2. Polymer Chemistry					
		3. Chemoinformatics					
		Organic Practicals – II	4	-	-	-	-
	Core Practicals	Inorganic Practicals – II	4	-	-	-	-
		Physical Practicals – II	4	-	-	-	-
	Core	Organic Chemistry – IV	4	4	50	50	100
<b>_</b>	Core	Inorganic Chemistry - IV	4	4	50	50	100
IV	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

Ready for

**Everv Good Work** 

NAAC 5<sup>th</sup> CYCLE

	Physical Practicals – II	4	4	50	50	100
HR	Human Rights	2	1	50	50	100

		Project Work	3	2	20	80	100
	Project				Viva	Thes	
						is	
	IDC	Advanced analytical		2*			
	IDC	technique/BMT					
	SCD	Chemical Sciences For CSIR-		2*			
	55F	UGC-NET/JRF/ GATE					
		Total	120	<b>90+6</b>			2200
l				*			

**Required Credits** = 9

= 90 (89 + 1 - HR)

#### Additional credits for Chemistry students - 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.	CH716	Organic Chemistry-I
2.	CH717	Inorganic Chemistry-I
3.	CH718	Physical Chemistry-I
4.	CH719A	Elective-I Analytical Chemistry
5.	CH719B	Elective-I Green Chemistry
6.	CH719C	Elective-I Pharmaceutical Chemistry
7.	CH818	Organic Chemistry-II
8.	CH819	Inorganic Chemistry-II
9.	CH820	Physical Chemistry-II
10.	CH821A	Elective-II Research Methodology
11.	CH821B	Elective-II Heterocyclic Chemistry
12.	CH821C	Elective-II Bio-Organic Chemistry
13.	PCH813	Organic Practicals-I
14.	PCH814	Inorganic Practicals-I
15.	PCH815	Physical Practicals-I

### Syllabus:

### SEMESTER I

### Organic Chemistry I

Course Code	CH716	Credit	4
Instruction Hours per Week	5	Marks	CIA (50) / SE (50)

**CRITERION I** 

Course Objective	<ul> <li>To know about the nature of aromaticity in the compounds</li> <li>To learn the kinetic and non-kinetic methods of determining organic reaction mechanism.</li> <li>To understand the substitution in aromatic and aliphatic reactions.</li> <li>To learn the addition and elimination reactions and their mechanisms</li> </ul>
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### **Course Outcomes:**

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

S.No	Course outcome	Cognitive
		level
CO-1	Define and distinguish the organic compounds based on the nature of aromaticity and characterizing them using NMR technique	(K1, K4)
CO-2	Interpret the intermediates involved in various organic reactions and integrate the kinetic and non-kinetic methods in determining organic reaction mechanism.	(K2, K3)
CO-3	Relate and categorize the nucleophilic substitutions in aromatic and aliphatic molecules with mechanism	(K2)
CO-4	Predict the product between electrophilic substitution in aromatic and aliphatic molecules reactivity and products formation with mechanism	(K5)
CO-5	Predictand write the addition and elimination reactions and their mechanisms	(K5, K6)
CO-6	Formulate the synthetic routes based on addition/elimination reactions in synthetic organic chemistry	(K6)

### Mapping of CO with PO and PSO

CO	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)						
CO	PO	PO	PO	PO	PO	PSO	PSO	PSO	PSO	PSO	PSO	Mean
	1	2	3	4	5	1	2	3	4	5	6	Score

**CRITERION I** 

												s of COs
- CO 1	3	3	2	2	1	3	3	3	3	3	2	2.5
- CO 2	3	3	3	2	1	3	3	3	3	2	2	2.5
- CO 3	3	3	2	2	1	3	3	3	3	3	2	2.5
- CO 4	3	3	3	2	1	3	3	3	3	3	3	2.7
- CO 5	3	3	3	3	1	3	3	3	3	3	2	2.7
- CO 6	3	3	2	3	1	3	3	3	2	3	2	2.5
Mean Overall Score									2.6			
Resu	lt											High

### **Assessment Pattern**

Bloom's Category	CA Tests (Marks Allotme	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: Aromaticity

Naming and numbering of alicyclic, bicyclic and tricyclic compounds (Basic skeletal structures only with or without one substituent). Concept of aromaticity and anti-aromaticity, delocalization of electrons -

Hückel's rule, criteria for aromaticity, examples of neutral and charged aromatic, non-aromatic, antiaromatic systems.

Aromaticity in charged rings and fused ring systems. - Benzenoid – Non-benzenoid aromatics – annulenes - NMR as a tool for aromaticity - anti- and homo-aromatic systems. Aromatic characterization of azulenes, tropones, annulenes and fullerenes.

### Unit - II: Reactive Intermediates and Methods of Determining Reaction Mechanism

Structure, stability, generation and reactions of Carbocations (classical and nonclassical), carbanions, carbenes, nitrenes and free-radicals.

Thermodynamic and Kinetic controlled reactions - non-kinetic methods - Product analysis and its importance Intermediates and Transition states- Trapping, testing and detection of intermediates-Cross over experiments. Isotopic labeling stereochemical studies.

Kinetic methods- Order-rate and rate constants-Energy of activation-entropy of activation-Influence of solvents, ionic strength, and salt and isotopic effects on the rate of the reaction.

### Unit - III: Aromatic and Aliphatic Electrophilic Substitution Reactions

Aromatic – Mechanism – Orientation and reactivity – Reactions: Nitrogen electrophiles: nitration, nitrosation and diazonium coupling - Sulphur electrophiles: sulphonation - Halogen electrophiles: chlorination and bromination - Carbon electrophiles: Friedel-Crafts alkylation, acylation and arylation reactions.

Aliphatic - Mechanisms:  $S_E2$ ,  $S_E1$  and  $S_{Ei}$ ; Substitution by double bond shifts; other mechanism: additionelimination and cyclic mechanism. Reactivity; Reactions: Hydrogen as electrophile: Hydrogen exchange; hydro-dehydrogenation; keto-enol tautomerism. - Halogen electrophiles: Halogenation of aldehydes and ketones; carboxylic acids - Nitrogen electrophiles: aliphatic diazonium coupling; direct formation of diazo compounds; direct amination; - sulphur electrophiles: sulphonation, - carbon electrophiles: acylation; alkoxy carbonyl alkylation; alkylation.

### Unit - IV: Aromatic and Aliphatic Nucleophilic Substitution Reactions

Aromatic -Mechanisms-  $S_NAr$ ,  $S_N1$  and Benzyne mechanisms. - Reactivity, Effect of structure, leaving group and attacking nucleophile.

Typical reactions: O and S-nucleophiles, Bucherer and Rosenmund reactions, von Richter, Sommelet-Hauser and Smiles rearrangements.

Aliphatic-Mechanisms-  $S_N1$ ,  $S_N2$ ,  $S_Ni$  and neighbouring group mechanisms. Nucleophilic substitutions at an allylic carbon, aliphatic trigonal carbon and vinyl carbon.

Reactivity: Effect of substrate, attacking nucleophile, leaving group and the medium - Swain-Scott, Grunwald-Winstein relationship - Ambident nucleophiles.

### **Unit - V: Addition and Elimination Reactions**

Additions-Addition to carbon-carbon multiple bonds-addition mechanisms-electrophilic, nucleophilic and free-radical additions cyclo addition-orientation and reactivity. Selected reactions – Birch reduction- Diels-Alder reaction- Hydroboration- Michael reaction. hydroxylation, 1,3-dipolar additions. -Simon Smith reaction, Mannich, Darzens, Wittig, Wittig-Horner, benzoin reactions and Cope eliminations..Stereochemical aspects of each reaction.

E1, E2, and E1cb mechanisms. - Syn Eliminations - E1-E2-E1cb spectrum - Orientation of the double bond: Hoffmann and Saytzeff rules. Reactivity: Effect of substrate, attacking bases, leaving group and medium. -Mechanisms and orientation in pyrolytic eliminations.

### References

- 1. R.O.C.Norman, Chapman, Organic Synthesis Prentice and Hall, NY, 1980.
- 2. Niel Isaacs, Physical Organic Chemistry, ELBS publications, 1987.
- 3. S.M.Mukherji and S.P.Singh, Organic Reaction Mechanism, MacMillan India Ltd., Chennai, 1990.
- 4. Francis A. Carey and Richard Sundberg, Advanced Organic Chemistry, Part A and B, , 3<sup>rd</sup> E dition, Plenum Press, 1990.
- 5. C Wentrup, Reactive Molecules, John Wiley and Sons, New York, 1984.
- 6. J.March, Advanced Organic Reaction mechanism and structure, Tata McGraw Hill, 2000.
- 7. V.K.Ahluwalia, Pooja Bhagat, Intermediates for Organic Synthesis, I.K International, 2005.
- 8. S.C.Pal, Nomenclature of organic compounds, Revised Edn. Narosa Publications, 2008.
- 9. Ahluwalia and Parashar, Organic Reaction Mechanisms, 4<sup>th</sup>Edn., Narosa Publications, 2012
- 10. P.S.Kalsi, Organic Reaction Mechanism, 3<sup>rd</sup>Edn. New Age Publications, 1994.

### **Online Resources:**

http://eacharya.inflibnet.ac.in/ Organic Chemistry- (Reaction Mechanisms-I)

### Syllabus:

### SEMESTER I

### Inorganic Chemistry-I

Course Code	CH717	Credit	4
Instruction Hours per Week	4	Marks	CIA (50) / SE (50)
Course Objective	<ul> <li>To impart the knowledge a their significance.</li> <li>To understand the theorie their importance.</li> <li>To study the basic chemis nano materials</li> </ul>	bout the struct s of coordina stry of rare ea	tion complexes and trin complexes and with elements and

### **Course Outcomes**

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

CO1	Gain knowledge about the structure and bonding of Inorganic compounds like	K1,
	polyacids, Inorganic Polymers, polysulphur – nitrogen and their significance	K2
CO2	Correlate the structure, bonding, stability and applications of metallocarboranes and Metal Clusters	K4
CO3	Relate and asses the applications of organometallic compounds in the field of synthetic chemistry and catalysis	K3, K5
CO4	Analyse the solid materials with defects that can be used in field of electronic industries foe designing energy materials.	K5
CO5	Understand the Solid-state Transformation, its thermodynamic, kinetics and nucleation in solid state materials	K2
CO6	Design and synthesis the energy producing nano materials and energy storage nanomaterials to meet the energy crisis in the future	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	3	2	3	3	2	3	2	2.7
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	3	3.0
4	3	3	3	3	3	3	3	3	3	3	3	3.0
5	3	3	3	3	2	2	3	3	3	3	2	2.7
6	3	3	3	3	3	3	3	3	3	3	2	2.9
									Mear	o Overall	Score	2.9
Result E										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: Structure and Bonding – I

Polyacids: Isopolyacids and hetereopolyacids of vanadium, chromium, molybdenum and Tungsten.Inorganic Polymers: Silicates, structure – properties – correlation and applications – molecular sieves, polysuphur – nitrogen compounds and poly organophosphazenes.

### Unit - II: Structure and Bonding – II

Boron hydrides: Polyhedral boranes, hydroboration, carboranes and metallocarboranes Metal Clusters: Chemistry of low molecularity metal clusters (upto) trinuclear metal Clusters: multiple metal-metal bonds.

### Unit - III: Solid State Chemistry – I

Introduction-Single and polycrystalline materials-Solid state Reactions-Co-precipitation as precursor to solid state reactions-Other Precursor Methods-Kinetics of solid-state reactions-Perfect and imperfect crystals. Defects in solids: Point defects-Schottky defects-Frenkeldefects.Thermodynamics of Schottky and Frenkel defect formation. Non-stoichiometric defects: metal excess and metal deficiency. Spinels-solid state lasers-inorganic phosphors-Ferrite.

#### Unit - IV:Solid State Chemistry - II

Colourcentres-Vacancies and interstitials in non-stoichiometric crystals. Extended defects –subgrain boundaries and antiphase domains-Solid state transformations-Classification of transformations-Thermal decomposition reactions-Laws governing nucleation-Crystal growth of nuclei-Reaction between two solids-polymorphism-Characterization and properties of polymorphs.

#### Unit - V: Chemistry of rare earths and nanomaterials

The Chemistry of solid state, lanthanides and actinides, oxidation state spectral, magnetic characteristics, coordination numbers, nuclear and non-nuclear applications.

Nanomaterials: General introduction - Synthesis of nanoparticles of gold and silver - Synthesis of nanoparticle semiconductors ( $TiO_2$  and  $Fe_2O_3$ ) - Nanowires and nanorods - Self-assembled nanostructures - Self-assembly and bottom-up fabrication – Graphenes, fullerenes and nanotubes - Applications of nanoparticles-application as sensors, biomedical applications, application in optics and electronics.

### **Text Books**

#### References

- 1. K.F. Purcell and J.C. Kotz, Inorganic Chemistry, WB Saunders Co., USA, 1977.
- 2. J.E. Huheey, Harper and Collins, Inorganic Chemistry, NY, IV Edition, 1993.
- 3. FA Cotton and G.W. Wilkinson, Advanced Inorganic Chemistry, A comprehensive Text, John Wiley and Sons, 1988.
- 4. B.E. Dogulas DH McDaniel's and Alexander Concepts and Models of Inorganic Chemistry, Oxford IBH, 1983.
- 5. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Univ. Science Books, 1994.
- 6. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life (An introduction and Guide), John Wiley & Sons, 1994.

- 7. WU. Mallik, G.D. Tuli, R.D. Madan, Selected topics in Inorganic Chemistry, S. Chand and Co., New Delhi, 1992.
- 8. A.R. West, Basic solid-state chemistry, John Wiley NY, 1991.
- 9. W.E. Addison, Structural principles in Inorganic chemistry, Longman, 1961.
- 10. D.M. Adams, Inorganic solids, John Wiley Sons, 1974.
- 11. J.N. Gurtu, Solid State Chemistry, Second Edition, PragatiPrakashan Publishers, 2015.
- 12. Dieter Vollath, Nanomaterials: An Introduction to Synthesis, Properties and Applications, 2nd Edition Wiley, 2013.
- 13. Zhong Cao G, "Nanostructures and Nanomaterials: Synthesis, Properties and Applications", Imperial College Press, London, United Kingdom, 2004

### **Online Resources**

1. http://eacharya.inflibnet.ac.in/ (Bioinorganic Chemistry-40 lectures)

### PHYSICAL CHEMISTRY I

Course Code	CH718	Credit	4
Instruction Hours per Week	4	Marks	CIA (50) / SE (50)
Course Objective	<ul> <li>To study the basic concept kinetics</li> <li>To illustrate the mechanicatalyzed reaction and their</li> <li>To apply and analyse the fast reactions by various m</li> <li>To learn and apply the stoperations in molecules</li> <li>To understand the concepts and find out the vibrational</li> <li>To construct the character for the stoperation of the</li></ul>	ts of various ism of acid r applications kinetics of co ethods. ymmetry ele s of selection l modes of the table for simp	theories in chemical h, base and enzyme momplex reactions and ments and symmetry rules in for transitions e molecules. ble molecules.

### **Course Outcomes**

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

CO. No.	Course Outcome Statement	Cognitive Level
CO 1	Understand the various theories of kinetics and compare their applications to reactions.	K1, K3
CO 2	Compare and contrast the different catalytic reaction and analyse their applications.	K2, K4
CO 3	Hypothesize mechanistic pathways for reactions based on the kinetic parameters.	K6
CO 4	Learn and sketch the different symmetry elements and evaluate the implications of symmetry operations in molecules.	K3, K5
CO 5	Assess the vibrational modes of molecules and thereby formulate the selection rules for transitions	K5, K6
CO 6	Develop the character table and analyse the symmetry operations of molecules	K4, K6

	Prog	ramme	Outco	omes (F	POs)	Programme Specific Outcomes (PSOs)						
CO	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	2	1	2.64
CO2	3	3	3	3	2	3	3	3	3	3	2	2.82
CO3	3	3	3	3	2	3	3	3	3	2	3	2.82
CO4	3	3	3	2	2	3	3	3	3	2	1	2.55
CO5	3	3	3	3	2	3	3	3	2	3	3	2.82
CO6	3	3	2	2	2	3	3	3	3	2	2	2.55
Mean Overall Score									2.70			
Result									High			

#### Assessment Pattern

Bloom's Category	CA Tests (Marks Allotme	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: Chemical Kinetics – I**

Collision theory, ARRT - partition function and activated complex - Eyring equation - estimation of free energy, enthalpy and entropy of activation and their significance - Theories of unimolecular gaseous reactions - RRK theory - limitations - RRKM theory. Reactions in solutions - effect of pressure, dielectric constant and ionic strength on reactions in solutions - kinetic isotope effects - linear free energy relationships - Hammett and Taft equations.

### **Unit - II: Chemical Kinetics – II**

Acid - Base catalysis - mechanism of acid - base catalyzed reactions - Bronsted catalysis law. Catalysis by enzymes - rate of enzyme catalyzed reactions - effect of substrate concentration, pH and temperature on enzyme catalyzed reactions - inhibition of enzyme catalyzed reactions, Michaelis-Menton equation - Autocatalysis and oscillatory reactions.

### **Unit - III: Chemical Kinetics – III**

Study of surfaces - Langmuir and BET adsorption isotherms-mechanism of heterogenous catalysis. Kinetics of complex reactions, reversible reactions, consecutive reactions, parallel reactions, chain reactions, general treatment of chain reactions - chain length - Rice Herzfeld mechanism - explosion limits. Study of fast reactions - relaxation methods - temperature and pressure jump methods-stopped flow and flash photolysis methods.

### **Unit - IV: Group Theory – I**

Symmetry elements and symmetry operation –group multiplication table-subgroups, similarity transformation and classes-identifications of symmetry operations and determination of point groups-Matrix representation of symmetry operations - reducible and irreducible representations – direct product representation-The great orthogonality theorem and its consequences.

#### **Unit - V: Group Theory – II**

Construction of character table for  $C_2V$  and  $C_3V$  - Mulliken symbols -application of group theory. -hybrid orbital in nonlinear molecules (CH<sub>4</sub>, XeF<sub>4</sub>, BF<sub>3</sub>, SF<sub>6</sub> and NH<sub>3</sub>). Determination of representations of vibrational modes in non-linear molecules (H<sub>2</sub>O, CH<sub>4</sub>, XeF<sub>4</sub>, BF<sub>3</sub>, SF<sub>6</sub> and NH<sub>3</sub>). Symmetry selection rules for infrared and Raman Spectra-Electronic Spectra of Ethylene and formaldehyde.

#### References

- 1. J. Rajaram and J.C. Kuriacose, Kinetics and Mechanism of Chemical Transformations. Mac Millan India Ltd, 1993.
- 2. R.J. Laidler, Chemical Kinetics, Harper and Row, New York, 1987.
- 3. K.V. Ramakrishnan and M.S. Gopinath, Group Theory in Chemistry, Vishal Publications, 1998.
- 4. K.V. Raman, Group Theory and its Applications to Chemistry, Tata Mc Graw Hill Publishing Co., 1990.
- 5. G.M. Barrow, Physical Chemistry, McGraw Hill, 1988.
- 6. R.G. Frost and Pearson, Kinetics and Mechanism, Wisely, New York, 1961.
- 7. F.A. Cotton, Chemical Applications of Group Theory, John Wiley and Sons inc., New York, 1971.
- 8. B.S. Garg, Chemical Applications of Molecular symmetry and Group Theory, Laxmi Publications/Triniti/Macmillan, 2012
- 9. S. Swarnalakshmi, Simple Approach to Group Theory in Chemistry, Universities Press, 2008

#### **Online Resources:**

- 1. <u>http://eacharya.inflibnet.ac.in/</u> Applications of molecular symmetry and group theory [31 lectures]
- 2. http://nptel.ac.in/courses/104104080/

### <u>Syllabus:</u>

### **SEMESTER-I**

### **ANALYTICAL CHEMISTRY**

Course Code	CH719A	Credit	4
Instruction Hours per	4	Marks	CIA (50) / SE
Week			(50)
Course Objective	<ul> <li>To study the different typ NMR spectroscopy and i</li> <li>To study the analytical applications.</li> </ul>	es of molecula ts applications techniques, in	ar spectroscopy and s nstrumentation and

### **Course Outcomes**

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

CO. No.	Course Outcome Statement	Cognitive Level
CO 1	Explain and evaluate the theory and principle of electro analytical techniques, various factors involved in analysis and its applications.	K1 & K5
CO 2	Understand the fundamentals of microwave spectroscopy and how to identify molecules using structural factors like moment of inertia and intermolecular distances.	K1 & K6
CO 3	Explore the vibrating diatomic molecule, the simple harmonic oscillator, the anharmonic oscillator, and their applications in spectroscopy.	K3 & K5
CO 4	Illustration of Infrared Spectroscopy - Group frequencies Rotational and Vibrational Raman	K3 & K4
CO 5	Application of advanced chromatographic separation technique principles for isolation and characterization of compounds.	K2 & K4
CO 6	Identify and structurally categorize new using X-ray diffraction. Analyze nanomaterials using advanced electron microscopy characterization techniques.	K2 & K6

### Mapping of CO with PO and PSO

**Programme Outcomes (POs)** СО

	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	Mean Scores of COs
CO1	3	3	3	3	2	3	2	3	3	3	2	2.73
CO2	3	3	3	3	2	3	3	3	3	3	2	2.82
CO3	3	3	2	3	2	3	3	3	3	2	2	2.64
CO4	3	3	3	3	2	3	3	3	3	3	3	2.91
CO5	3	3	3	3	2	3	3	2	3	3	3	2.82
CO6	3	3	3	3	2	3	3	3	2	3	3	2.82
Mean Overall Score								2.79				
Result								High				

### **Assessment Pattern**

Bloom's Category	CA Tests (Marks Allotm	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: Polarography and Amperometry

Polarography – theory, apparatus, DME, Diffusion, Kinetic and catalytic currents, Current- Voltage curves for reversible and irreversible system; Qualitative and quantitative applications to inorganic and organic systems. Principle and Instrumentation of Cyclic Voltammetry. Stripping analysis-Anodic and Cathodic Stripping-Modified electrodes-need- fabrication-applications. Amperometry- principle- curves in amperometric titrations, apparatus, advantages of rotating platinum electrode and advantages of biamperometric titrations.

### Unit - II: Chromatographic Techniques

Gas liquid Chromatography - principle, Retention Volume, Relationship between Vg and K- Effect of mobile phase flow rate. Instrumentation-Carrier gas, sample injection system, column configurations and column ovens, Detectors systems FID and TCD. Column and stationary Phases-Open and tubular column, packed column, Stationary Phase. Applications of GLC. HPLC – principle, Scope, column efficiency, instrumentation, pumping system, column packing, detectors and applications.

### **Unit - III: Spectroscopy – I**

Electronic spectroscopy -selection rules-types of transition solvent effects.

Spin Resonance spectroscopy-origin of NMR signals, chemical shift-factors affecting chemical shift, spin spin coupling-NMR of simple AX and AMX type molecules-<sup>13</sup>C, <sup>19</sup>F, <sup>31</sup>P NMR spectra-applications-a brief discussion of Fourier transformation resonance spectroscopy.

### Unit - IV: Spectroscopy- II

Interaction of matter with radiation-Rotational spectroscopy of a rigid and non-rigid diatomic rotors-and polyatomic molecules-vibrational spectroscopy of harmonic and anharmonic oscillators and polyatomic molecules-overtones-fermi resonance and combination of bands- group frequencies –Raman spectroscopy- classical and quantum theories-

Rotational and vibrational Raman spectra- spectra of diatomic molecules-frank condon principle- Morse function. Polyatomic molecules, types of transition, solvent effects.

### Unit - V: XRD and Microscopic Techniques

X-ray diffraction- The laue method-the rotating crystal method- the powder method – the powder method – determination of grain size/ crystallite size using X-ray line broadening studies (Scherrer's formula) - Determination of crystallite size distribution using X-ray line shape analysis- X-ray diffraction pattern and analysis of same commercially important oxides – small angle X-ray scattering (SAXS).

Electron microscopy- Principle and instrumentation –Applications of scanning electron microscope (SEM)- Energy dispersive X-ray analysis (EDX)- Transmission electron microscope (TEM)- Scanning tunnelling microscope (STM)-Atomic force microscope (AFM).

### **15 Hours**

#### **15 Hours**

### **15 Hours**

**15 Hours** 

### **15 Hours**

#### References

- 1. D.A.Skoog, D.M. West and F. J. Holler, Analytical Chemistry an Introduction, Saunders College Publishers, 1990.
- 2. J. Mendham, R.C. Denney, J.D. Barnes and M. Thomas, Vogel's Text book of Quantitative
- 3. Chemical Analysis, Pearson Education Pvt. Ltd..2004.
- 4. J.G. Dick, Analytical Chemistry.Sir George Williams University, McGraw-Hill
- 5. Book Company, New. York. 1973.
- 6. H.H. Willard, L.L. Merritt, J.A. Dean and F.A. Seattle, *Instrumental methods of analysis*, 5thEdn., Harcourt Asia Pvt. Ltd., India, 2001.
- 7. Fundamentals of Molecular spectroscopy .by C.N.Banwell and E.M.Mccash, IV Edition, Tata McGraw Hill, 2005.
- 8. Vibrational Spectroscopy, by D.N.Sathyanarayana, New Age International Publishers, 2004.
- 9. Introduction.to Magnetic Resonance by Carington and Ad.Mclachlan, Harper and Row, New York, 1967.

### <u>Syllabus</u>

### **SEMESTER-I**

### **GREEN CHEMISTRY**

Course Code	CH719B	Credit	4
Instruction Hours per Week	4	Marks	CIA (50) / SE (50)
Course Objective	<ul> <li>To know eco-friendly me</li> <li>Understanding the synt compounds with the rev</li> </ul>	thods of synth- hesis of any rolution of Gre	esis. 7 type of organic 2 ten Chemistry

#### **Course Outcomes**

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

CO. No.	Course Outcome Statement	Cognitive Level
CO 1	Understand and compare the eco-friendly methods of synthesis.	K1, K2
CO 2	Appraising the measurement, Prevention and control of life-cycle assessment	K4
CO 3	Relate and asses the Renewable energy as Biomass, Fossil Fuels, solar energy and some other natural chemical resources.	K3, K5
CO 4	Analyse the organic compounds which found in application of green synthesis with the revolution of Green Chemistry.	K5
CO 5	Compare and analyze Green Technology and Alternative Energy Sources such as Microwaves, Electrochemical synthesis	K2
CO 6	Design the next generation agrochemicals and Industrial Case Studies from natures, using green reagents and bio catalyst.	К6

## Mapping of CO with PO and PSO

	Programme Outcomes (POs)					Progra	Programme Specific Outcomes (PSOs)					
СО	PO 1	PO 2	PO 3	PO 4	PO 5	PSO 1	PSO 2	PSO 3	PSO 4	PSO 5	PSO 6	Mean Score s of COs
- CO 1	3	3	2	3	3	3	3	2	3	3	3	2.82
- CO 2	3	3	2	2	3	3	2	3	3	2	3	2.64
- CO 3	3	3	3	3	3	3	2	3	3	3	3	2.91
- CO 4	3	3	3	2	3	3	3	2	3	3	3	2.82
- CO 5	3	3	3	3	3	3	2	3	3	3	3	2.91
- CO 6	3	3	3	3	3	3	3	3	2	3	3	2.91
Mean Overall Score							2.83					
Result										High		

### **Assessment Pattern**

Bloom's Category	CA Tests (Marks Allotme	ent)	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: Principles & Concept of Green Chemistry

Introduction –Concept and Principles-development of Green Chemistry- Atom economy reactions – rearrangement reactions, addition reactions- atom uneconomic-sublimation-elimination-Wittig reactions- toxicity measures- Need of Green Chemistry in our day-to-day life.

### Unit - II: Measuring and Controlling Environmental Performance

Importance of measurement – lactic acid production-safer Gasoline – introduction to life cycle assessment-four stages of Life Cycle Assessment (LCA) –Carbon foot printing-green process Matrics-eco labels - Integrated Pollution and Prevention and Control (IPPC)-REACH (Registration, Evaluation, Authorization of Chemicals).

### Unit - III: Emerging Green Technology and Alternative Energy Sources 15 Hours

Design for Energy Efficiency-Photochemical reactions- Advantages-Challenge faced by photochemical process. Microwave technology on Chemistry- Microwave heating –Microwave assisted reactions-Sono chemistry and Green Chemistry –Electrochemical Synthesis-Examples of Electrochemical synthesis.

### **Unit - IV: Renewable Resources**

Biomass –Renewable energy – Fossil Fuels-Energy from Biomass-Solar Power- Other forms of renewable energy-Fuel Cells-Alternative Economics-Syngas economy- hydrogen economy-Bio refinery chemicals from fatty acids-Polymer from Renewable Resources –Some other natural chemical resources.

### **Unit - V: Industrial Case Studies**

Methyl Methacrylate (MMA)-Greening of Acetic acid manufacture-Vitamin C-Leather manufacture – Types of Leather –Difference between Hide and Skin-Tanning –Reverse tanning –Vegetable tanning – Chrome Tanning-Fat liquoring –Dyeing –Application-Polyethylene- Ziegler Natta Catalysis-Metallocene Catalysis-Eco friendly Pesticides-Insecticides.

#### References

- 1. Mike Lancaster, Green Chemistry and Introductory text, II Edition, 2003.
- 2. P.T.Anastas and J.C Warner, Green Chemistry theory and Practice, Oxford University press, Oxford, 1988..
- 3. P.Tundoet. al., Green Chemistry, Wiley –Blackwell, London, 2007.
- 4. V.K. Ahluwalia, Environmental chemistry, Ane Books, India, 2003.
- 5. T.E Graedel, Streamlined Life cycle Assessment, Prentice Hall, NewJersey, 1998.
- 6. V.K. Ahluwalia, Methods and Reagents of Green Chemistry: An Introduction to Green Chemistry, 2013.

### **Online Resource**

www.clri.org.

### Syllabus:

### **SEMESTER-I**

### CH719C – PHARMACEUTICAL CHEMISTRY

Course Code	СН719С	Credit	4
Instruction Hours per Week	4	Marks	CIA (50) / SE (50)
Course Objective	<ul><li>To understand the compo</li><li>To know the different typ</li></ul>	sition and the bes of drugs an	kinetics of drugs ad its composition

### **Course Outcomes**

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

CO. No.	Course Outcome Statement	Cognitive Level
CO 1	Learn the terminologies and mechanism of action of drugs and analyse them	K1& K4
CO 2	Discuss about the different types of drugs and their applications and evaluate their structures	K2 & K5
CO 3	Explain the causes of certain ailments and treatment and relate them	K2 & K3
CO 4	Understand the extraction and uses of some specific drugs and categorize them	K1 & K4
CO 5	Enumerate various therapeutic agents and combine them for potential applications	K1 &K6
CO 6	Tabulate the various hematological factors assess their effects on human body	K1 & K5

### Mapping of CO with PO and PSO

	Programme Outcomes (POs)					Progra	Programme Specific Outcomes (PSOs)					
со	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	Mean Scores of COs
C01	3	3	3	3	2	3	3	3	2	3	3	2.82
CO2	3	3	3	3	3	3	3	2	3	3	3	2.91
CO3	3	3	2	2	3	3	2	3	3	3	3	2.73
CO4	3	3	3	2	3	3	3	2	3	3	3	2.82
CO5	3	3	3	3	3	3	3	3	2	3	3	2.91
CO6	3	3	3	2	3	3	2	3	3	2	3	2.73
Mean Overall Score									2.82			
Result										High		

#### **Assessment Pattern**

Bloom's Category	CA Tests (Marks Allotme	ent)	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: Introduction**

Importance of chemistry in pharmacy, important terminologies used their meaning- molecular pharmacology, pharmacodynamics, pharmacophore, metabolites, virus antimetabolites, bacteria, fungi, actinomycetes.

Mechanism of action of drug types: assay- biological, chemical immunological-statement only. Mechanism: metabolism of drugs and their effect on pharmacological activity. Absorption of drugs. Drug delivery system, sustained release of drugs. Physiological effects of different functional groups in drugs. Testing of potential of drugs and their side effects. Indian medicinal plants and trees-adathode, tulsi, thoothuvalai, shoeflower, fia, neem, mango, kizhanelliocimum,grass and greens. Causes and symptoms of common diseases- tuberculosis, asthma, jaundice, piles,leprosy,epilepsy,typhoid,malaria, cholera, filarial.

### **Unit - II: Antibiotics and Vitamins**

Antibiotics: definition, structure, uses of chloramphenicolampicillin, streptomycin, tetracycline, rifamycin Macrolides-Erythromycin-properties and uses.

Structural features-SAR functional group responsible for drug action, structural modification that changes the potency of the above drugs. Conditions for their use as therapeutic agents. Fields of application.Sulphonamides: substituents in the amide group. General properties and drug action. Preparation and uses of sulphadiazin, sulphapyridine, sulphathiazole, sulphafurazole and prontosil. Vitamins: classification. Role in Chemotherapy. Uses. Deficiency and symptoms. Estimation of vitamins A,  $B_1$ ,  $B_2$  and C.

#### Unit - III: Antipyretic, analgesics, anti-inflammatory agents

Classification: action of analgesics. Narcotic analgesics: Morphine and its derivatives. SAR. Synthetic analgesics-pethidine and methadones. Salicylic acid and its derivatives, indolyl derivatives, aryl-acetic acid derivatives, pyrazole, p-aminophenol derivatives-mechanism of action. Antiseptics and disinfectants: definition, standardization of disinfectants. Use of phenols, dyes, chloramines, chlorhexadiene, organomercurials. Dequalinium chloride, formaldehyde, cationic surface-active reagents, chloraminet-nitrofurazone. Distinction between antiseptics and disinfectants. Anaesthetics: definition, classification. Uses of volatile anaesthetics- nitrous oxide, ethers, cyclopropane, chloroform, halothane, trichlorethlene.

#### **Unit - IV: Alkaloids**

Alkaloids: sources, isolation and purification, colour reactions and detection general. Quinine and Morphine- sources, extraction, structure, important features and SAR. Tranquilisers, sedatives, hypnotics, psychedelic drugs. Organic pharmaceutical aids: role as preservatives, antioxidants, colouring, flavouring, sweetening, emulsifying agents, stabilizing and suspending agents. Ointment bases. Solvents. Minerals: biological role of salts of Na, K and Ca, trace elements Cu, Zn and I. deficiency. Sources. Diagnostic agents: organic types for different actions, examples.

### Unit: V Blood and Haematological agents

Blood: composition.Analysis of blood sample-grouping, Rh factor. Tests for urea, bile carbonyls compounds, serum and protein in a sample. Physiological function of plasma protein. Roel of blood as oxygen carrier. Structure of heme. Clotting mechanisms. Factors involved. Blood pressure-normal, low and high – causes and control, anemia causes, detection. Antianemic drugs.

Haematological agents: coagulants and anticoagulants. Coagulants-vitaminK, Protamine, sulphate, dried thrombin, proteins, amino acids, anti-coagulants- coumarins, indanedioals, citric acid, 2-sulphonyloacids, quinoxaline, thromlodyn, haemostatics, amino-caproic acid, tranexamic acid, anemia: causes, detection, antianemic drugs.

#### References

- 1. Charles R. Craig, Robert E. Stitzel, Modern Pharmacology, 3<sup>rd</sup> edition, little brown and company, Boston, 1990.
- 2. Saradasubrahmanyam, K. Madhavankulty, Textbook of human physiology, 4<sup>th</sup> edition, S.Chand and company Ltd., New Delhi, 1995.
- 3. G.R.Chatwal, pharmaceutical chemistry, Vol.II, 1<sup>st</sup> edition, Himalaya Publishing House, Bombay, 1991.
- 4. Harold Varley, Practical clinical biochemistry, 4<sup>th</sup> edition, Arnold-Heinemann, New Delhi,1976. Jacques Wallach, Interpretation of Diagnostic Tests, Little Brown and Company, Boston, 1992.

Semester-II

### Organic Chemistry II

Course Code	CH818		Credit	4
Instruction Hours per Week	4		Marks	CIA (50) / SE (50)
Course Objective	•	To understand the add oxidation reaction mech To learn the concept of of organic molecules.	lition, elimina nanisms f bonding, stru	tion, reduction and

### **Course Outcomes:**

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

S.No	Course outcome	Cognitive level
CO-1	Define the concept of chirality and categorize the structure of organic molecules through stereo isomerism and various molecular 3D-models and stereochemical rules	(K1, K2, K4)
CO-2	Annotate and integrate the conformations and reactivity, chirality concepts involved in cyclic, acyclic, bicyclic systems	(K2, K3)
CO-3	Relate the product formation from various oxidation reactions and various oxidizing reagents with detailed mechanism	(K2)
CO-4	Write and justify the product of reduction reactions and various reducing reagents with detailed mechanism.	(K3, K6)
CO-5	Illustrate the various selective naming reactions with mechanistic route and predict the product formation	(K3,K5)
CO-6	Justify the synthetic organic chemistry problems and predict the product with specific stereochemistry in oxidation, reduction and selective naming reactions	(K3)

### Mapping of CO with PO and PSO

	Programme (POs)		Outcomes		Progr	Programme Specific Outcomes (PSOs)				Os)		
СО	PO 1	PO 2	PO 3	PO 4	PO 5	PSO 1	PSO 2	PSO 3	PSO 4	PSO 5	PSO 6	Mean Score s of COs
- CO 1	2	3	2	3	1	3	2	3	2	3	3	2.5
- CO 2	3	3	3	2	1	3	3	3	2	2	2	2.5
- CO 3	3	3	3	3	1	3	3	3	3	3	2	2.7
- CO 4	3	3	3	3	1	3	3	3	3	3	2	2.7
- CO 5	3	3	3	2	1	3	3	3	2	2	3	2.5
- CO 6	3	3	2	2	1	3	3	3	2	3	3	2.5
Mean Overall Score								2.6				
Result									High			

### **Assessment Pattern**

Bloom's Category	CA Tests (Marks Allotme	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: Stereochemistry – I

Introduction to molecular symmetry and chirality – examples from common objects to molecules – axis, plane, center, alternating axis of symmetry. Stereoisomerism – definition based on symmetry and energy criteria – configuration and conformational stereoisomers.

Chirality – molecules with C, N, S based chiral centers – absolute configuration - enantiomers – racemic modifications - R and S nomenclature using Cahn-Ingold-Prelog rules – molecules with a chiral center and Cn – molecules with more than one center of chirality – definition of diastereoisomers – constitutionally symmetrical and unsymmetrical chiral molecules - erythro, threo nomenclature – E and Z nomenclature. Asymmetry synthesis - Cram's rule – Optical and geometrical isomerism of disubstituted cycloalkanes-Stereoselective and stereospecific synthesis.

### Unit - II: Stereochemistry – II

Axial, planar and helical chirality – examples – stereochemistry and absolute configuration of allenes, biphenyls, trans cyclooctene, transcyclononene and binaphthyls, ansa and cyclophanic compounds, spiranes, exo-cyclic alkylidene cycloalkanes.

Topicity and prostereoisomerism – topicity of ligands and faces, and their nomenclature – NMR distinction of enantiotopic/diastereotopic ligands. Conformational analysis and stereochemical features of acyclic and cyclic systems – substituted n-butanes – cyclohexane and its derivatives – decalins – fused and bridged bicyclic systems – conformation and reactivity - some examples – chemical consequence of conformational equilibrium - Curtin-Hammett principle.

### Unit - III: Selected Organic Name Reactions with Mechanism

Arbuzov reaction, Barmford-stevens reaction, Duff reaction, Claisen condensation, Stork Enamine reaction, Hunsdieker,Ulmannraction, Swern Oxidation, Kolbe reaction, Meerweinarylation, Hofmann-Loffler-Fretag, Peterson olefination, and Chugaev reaction. Wohl-zieglerbromination, Stephen reaction, Schotten-Baumann reaction, Suzuki reaction. Stereochemical aspects of each reaction. Stereochemical aspects of each reaction.

### **Unit - IV: Oxidation Reactions**

Metal based and non-metal-based oxidations of alcohols to carbonyls (Chromium, Manganese, aluminium, silver, and ruthenium. DMSO, hypervalent iodine and TEMPOL based reagents). Phenols (Fremy's salt, silver carbonate). Alkenes to epoxides: (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation. Alkenes todiols: (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification. Alkenes to carbonyls with bond cleavage (Manganese, Osmium, Ruthenium and lead based, ozonolysis). Alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, selenium, chromium based allylic oxidation) - ketones to ester/lactones (Baeyer-Villiger).

#### **Unit - V: Reduction Reactions**

Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium/Nickel etc; Homogeneous: Wilkinson). Noyori asymmetric hydrogenation. Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium, Zinc, Titanium and Samarium (Birch, Pinacol formation, McMurry, Acyloin formation, dehalogenation and deoxygenations) - Hydride transfer reagents from Group III and Group IV in reductions. - NaBH<sub>4</sub> triacetoxyborohydride, L-selectride, K-selectride, Luche reduction; LiAlH<sub>4</sub>, DIBAL-H, and Red-Al,Trialkylsilanes and Trialkylstannane, Meerwein-Pondorff-Verley reduction) - Stereoselective and enantioselective reductions (Chiral Boranes, Corey-Bakshi-Shibata).

#### References

- 1. Francis A. Carey and Richard J, Sundberg, Advanced Organic Chemistry Part B, 3<sup>rd</sup> Edition 1990.
- 2. S.M. Mukherji and S.P. Singh, Organic Reaction Mechanism, MacMillan India Ltd., Chennai 1990.
- 3. P.S. Kalsi, Stereochemistry and Mechanism through solved problems, Wiley Eastern Ltd., 1994.
- 4. W Carruthers, Some Modern Methods of Organic Synthesis, 4<sup>th</sup>Edn. Edition, Cambridge University Press, 1996.
- 5. H.O. House, Modern Synthetic Reactions, The Benjamin Cummings Publishing Company, London, 1972.
- 6. P.S.Kalsi, Stereochemistry, Conformation analysis and Mechanism by 2<sup>nd</sup> Edition Wiley Eastern Limited , 1993.
- 7. Ernest Eliel, Stereochemistry of carbon compounds, New Age Publications, 2012.
- 8. D.Nasipuri, Sterochemistry of Organic compounds, 2<sup>nd</sup>Edn. New Age Publications,
- 9. 2008.
- 10. J.March, Advanced Organic Reaction mechanism and structure, Tata McGraw Hill, 2000.
- 11. Ahluwalia and Parashar, Organic Reaction Mechanisms, 4th Edn., Narosa Publications, 2012
- 12. P.S.Kalsi, Organic Reaction Mechanism, 3<sup>rd</sup>Edn. New Age Publications, 1994.

#### **Online resources:**

1. http://eacharya.inflibnet.ac.in/ Organic Chemistry- (Reaction Mechanisms-II)

### **SEMESTER-II**

### Inorganic Chemistry-II

Course Code	CH819	Credit	4					
Instruction Hours per Week	4	Marks	CIA (50) / SE (50)					
Course Objective	<ul> <li>To study the concept o of the complexes and s</li> <li>To study about struct complexes.</li> <li>To learn the use of In</li> </ul>	<ul> <li>To study the concept of coordination Chemistry, stab of the complexes and stereochemistry of complexes.</li> <li>To study about structure and bonding in coordina complexes.</li> </ul>						
	<ul> <li>systems</li> <li>To study the electron treactions in Coordination</li> </ul>	sses and substitution						

### **Course Outcomes**

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

CO1	Deduce the reaction mechanism and stability of the coordination compounds	K5
CO2	Understand the theories of coordination compounds and relate their importance.	K2, K3
CO3	Know the basic chemistry of various elements and their functions in biological systems	K1
CO4	Comprehend and integrating the role of coordination compound in living system	K4
CO5	Analyse the basic application of electronic spectroscopy of complexes and apprise the stability of coordination compounds	K5
CO6	Design and synthesis coordination compounds of biological and medicinal importance	K6

Mapping of CO with PO and PSO

СО	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	3	3	3	3	3	3	2	2.9
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	3	2	3	3	3	3	2	2.8
5	3	3	3	3	3	3	3	3	2	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 Allotme	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: Coordination Chemistry – I

Thermodynamic aspects of complex formation; Stability of complexes, factors affecting stability, Determination of stability constants by spectrophotometric, polarographic and potentiomteric methods. Electronic spectroscopic studies of coordination complexes.

### **Unit - II: Coordination Chemistry – II**

Stereochemical aspects; Stereoisomerism in inorganic compelexes; isomerism arising out of ligand and ligand conformation; chirality and nonmenclature of chiral complexes; optical rotatory dispersion and circular dichroism, Absolute configuration, Cotton effect.

Macrocyclic. Ligands; types; porphyrins; corrins, Schiff bases; crown ethers; cryptates

### Unit - III: Bio-Inorganic Chemistry – I

Transition elements in biology - their occurrence and function, active-site structure and function of metalloproteins and metalloenzymes with various transition metal ions (carbonic anhydrase and carboxy peptidase) and ligand systems;  $O_2$  binding properties of heme (haemoglobin and myoglobin) and non-heme proteins hemocyanin & hemerythrin), their coordination geometry and electronic structure, co-operativity effect, Hill coefficient and Bohr Effect. Na-K pump.

#### **Unit - IV: Coordination Chemistry – III**

Electron transfer reactions, outer and inner sphere processes, atom transfer reaction, formation and rearrangement of precursor complexes, the binding ligand, successor complexes, Marcus Theory. Complementary, non-complementary and two electron transfer reactions.

#### Unit - V: Coordination Chemistry - IV

Substitution Reaction: Substitution in square planar complexes, reactivity of platinum complexes, influences of entering, leaving and other groups. The trans effect, Theories of trans effect and its applications. Substitution of octahedral complexes of cobalt and chromium, replacement of coordinated water, solvolytic (acids and bases) reaction applications in synthesis (Platinum and cobalt complexes only).

#### **Text Books**

#### References

- 1. J.E. Huheey, Inorganic Chemistry Principles, Structure and Reactivity, Harper Collins, New York, IV Edition, 1993.
- 2. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry A Comprehensive Text, John Wiley and Sons, V Edition, 1988.
- 3. K.F. Purcell and J.C. Kotz, Inorganic Chemistry WB Saunders Co., USA, 1977.
- 4. M.C. Day and J. Selbin, Theoretical Inorganic Chemistry, Van Nostrand Co., New York, 1974.
- 5. D.F. Shrivers, P.W. Atkins and C.H. Langford, Inorganic Chemistry, OUP, 1990,
- 6. S.F.A.Kettle, Coordination Chemistry, EIBS, 1973.
- 7. K. Burger, Coordination Chemistry, Burter. Worthy, 1973.
- 8. F. Basolo and R.G. Pearson, Mechanism of Inorganic Reaction, Wiley NY, 1967.

#### **Online Resource:**

http://nptel.ac.in/courses/104105033/ Coordination chemistry (Chemistry of transition elements )

### Syllabus:

### **SEMESTER-II**

### CH820 PHYSICAL CHEMISTRY II

Course Code	CH820	Credit	4
Instruction Hours per Week	4	Marks	CIA (50) / SE (50)
Course Objective	<ul> <li>To study and apply the quantum mechanics in cher</li> <li>To illustrate the physical s and Schrodinger equation</li> <li>To learn and analyse the pr molar property and fugacity</li> <li>To learn the fundamental thermodynamics.</li> <li>To understand and assess th – equilibrium thermodynam</li> <li>To apply non – equilibrium biological systems.</li> </ul>	fundamentals nistry ignificance of inciples and si 7. Is and applica the concepts of nics in various thermodynan	and principles of the wave functions gnificance of partial ations of statistical equilibrium and non phenomenon. hics to chemical and

### **Course Outcomes**

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

CO. No.	Course Outcome Statement	Cognitive Level
CO 1	Understand and explain the principles of quantum mechanics and apply it to chemical systems.	K1, K3
CO 2	Describe the physical significance of the wave functions and apply the Schrödinger equation for some simple systems	K2, K3
CO 3	Understand the concepts and significance of thermodynamics and evaluate their applicability to chemical systems.	K1, K5
CO 4	Assess the different statistical approaches to chemical system and evaluate the thermodynamic quantities in terms of partition function.	К5
CO 5	Recognize the principles that govern equilibrium and non- equilibrium thermodynamics and analyse the impact on non- equilibrium thermodynamics in electrokinetic and thermoelectric phenomenon	K1, K4
CO 6	Integrate the concepts and its implications of non – equilibrium thermodynamics to chemical and biological systems	K3, K6

## Mapping of CO with PO and PSO

	Programme Outcomes (POs)					Progra	Programme Specific Outcomes (PSOs)					
СО	PO 1	PO 2	PO 3	PO 4	PO 5	PSO 1	PSO 2	PSO 3	PSO 4	PSO 5	PSO 6	Mean Score s of COs
- CO 1	3	3	3	3	2	3	3	3	3	2	1	2.64
- CO 2	3	3	2	2	2	3	3	3	3	2	2	2.55
- CO 3	3	3	3	3	3	3	3	3	2	2	2	2.73
- CO 4	3	3	3	3	2	3	3	3	3	2	2	2.73
- CO 5	3	3	2	3	2	3	3	3	3	3	2	2.73
- CO 6	3	3	3	3	2	3	3	3	3	3	2	2.82
Mean Overall Score								2.70				
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: Introduction to Quantum Chemistry

Need for quantum mechanics. Black body radiation, photoelectric effect, Wave -particle dualism, Compton effect- Bohr's theory for hydrogen atom - Radius of Stationary Orbits-Energy of Electron in a Stationary Orbit-Heisenburg uncertainty principle and its applications

Solving One-dimensional wave equation for a standing wave-Separation of variables- Interpretation of results-Schrodinger's wave equation-Eigen value-Eigen function.

Postulates of Quantum mechanics –Normalization of wave functions, orthogonality of wave functions -Operators – Algebra of operators – commutative property – Linear operator and Hermitian property -Properties of Hermitian Operator– momentum operator, KE operator, Hamiltonian operator.

Solution of Schrodinger's wave equation for simple systems: Free particle- Particle in one dimensional box (Origin of quantization)

### Unit - II: Quantum mechanics to simple systems in chemistry

Particle in one dimensional box (Expectation Values for momentum and position meaning of  $\langle x \rangle$ ,  $\langle p \rangle$ , Verification of Heisenberg's Uncertainty Principle) -Applications of particle in a box -and particle in three-dimensional (3D) box.

Harmonic oscillator-interpretation of results, Rigid rotor-interpretation of result-angularmomentum operator

Hydrogen atom-Hydrogen atomic orbitals-Analytical and graphical representations

Radial probability distribution function-Orthogonality of 1s, 2s, 2p orbitals

Pauli's exclusion principle, Slater's determinant. Introduction to perturbation and Variational method (Qualitative)

### Unit - III: Thermodynamics

Partial molar properties – Partial molar free energy (Chemical potential) – Partial molar volume and partial molar heat content – their significance and determination of these quantities. Gibbs-Duhem equation-variation of chemical potential with temperature and pressure.

Thermodynamics of real gases – gas mixture – fugacity definition Gibbs-Duhem-Marghules equation– determination of fugacityby graphical and equation of state – variation of fugacity with temperature and pressure – thermodynamics of ideal and non - ideal binary solutions-dilute solutions- the concepts of activity and activity coefficients-determination of standard free energies. Choice of standard states – determination of activity and activity coefficients for non-electrolytes.

### **Unit IV: Statistical thermodynamics – I**

Statistical mechanics of a system of independent particles – Bose – Einstein system and Fermi Dirac systems. Distribution laws – Boltzmann Distribution law – Partition function and its significance. Bose – Einstein and Fermi Dirac Distribution law.

Limit of applicability of distribution law. Relationship between partition and thermodynamic functions – Internal energy, Heat capacity, Entropy, Pressure and Chemical potential.

Distribution law of distinguishable and indistinguishable molecules or particles –Thermodynamic quantities in terms of partition function. Evaluation of independent molecular function – Translational, rotational and vibrational – the law of equipartition energy – Heat capacity.

### Unit V: Application of Statistical and Irreversible thermodynamics:

Application of statistical to ideal monoatomic and Diatomic ideal gases. Heat capacity and the residual entropies of gases. Heat capacity of solids.Maxwell-Boltzmann probability distribution of molecular velocities and speeds. The concept of ensemble, Treatment of canonical ensemble, expression of entropy, enthalpy, Helmholtz free energy.

Near equilibrium process: General theory- Conservation of mass and energy- Entropy

production in open system by (i) heat (ii) matter and (iii) current flow. Onsager theory: Validity and verification. Thermoelectricity-Electro kinetic and thermo mechanical effects. Application of irreversible thermodynamics to biological and non-linear systems.

### References

- 1. Donald A McQuarrie, Quantum chemistry, Indian Edition, Viva Books Private Limited 2005
- 2. K.L. Kapoor, A text book of Physical Chemistry, Vol 4, Mac Millan India Ltd., 2001.
- 3. Prasad R.K. Quantum Chemistry, 1st Edition, New Delhi, Wiley Eastern Ltd, 1992.
- 4. M.C.Gupta, Statistical thermodynamics Second edition, Wiley Easter, New Delhi, 1990.
- 5. S. Glasstone, Thermodynamics for chemists, Affiliated East West Press, New Delhi, 1960
- 6. Francis W. Sears, Gerhard L. Salinger. Thermodynamics, Kinetic theory and Statistical thermodynamics. Addison Wesley (1975)
- 7. J. Rajaram and J.C. Kuriacose, Thermodynamics for students of chemistry, Lal Nagin Chand, New Delhi, 1986
- 8. K.L. Kapoor, A text book of Physical Chemistry, Vol 5, Mac Millan India Ltd., 2015.

#### **Online Resources**

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

### <u>Syllabus</u>

### **SEMESTER-II**

### CH821A RESEARCH METHODOLOGY

Course Code	C327	Credit	4
Instruction Hours per Week	4	Marks	CIA (50) / SE (50)
Course Objective	<ul> <li>To learn the purpose and m</li> <li>To study the interpretation literature search</li> <li>To write a scientific report</li> </ul>	ethods of rese of knowledge based on the r	arch of e-sources in esearch done

### **Course Outcomes**

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

CO. No.	Course Outcome Statement	Cognitive Level
CO 1	Understanding the importance of the research and to demonstrate high ethical values in research	K1, K6
CO 2	Employ different methodologies to conduct a literature survey	К3
CO 3	Analyse and execute a proper literature survey for a chosen problem in their respective field of research	K4, K5
CO 4	Integrating various level of hypothesis in analysing the data obtained during the research and interpret them	K4
CO 5	Organizing and evaluating the data obtained using various software's	K2, K4
CO 6	Compile a research article using the art of technical writing and subsequently publish	K6

### Mapping of CO with PO and PSO

	Prog	ramme	Outco	omes (F	POs)	Progra	Programme Specific Outcomes (PSOs)					
со	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	Mean Scores of COs
CO1	3	2	2	3	3	3	2	2	3	3	2	2.55
CO2	3	3	2	3	2	3	2	2	3	3	3	2.64
CO3	3	3	3	2	3	3	2	3	3	3	3	2.82
CO4	3	3	3	3	2	3	2	3	3	3	3	2.82
CO5	3	2	3	3	3	3	3	2	2	3	3	2.73
CO6	3	3	3	3	3	3	2	2	3	3	3	2.82
Mean Overall Score									2.73			
Resul	Result									High		

### **Assessment Pattern**

Bloom's Category	CA Tests (Marks Allotme	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 Introduction**

Meaning of Research, Objectives of Research, Motivation in Research, Types of Research, Research Approaches, Significance of Research, Research Methods versus Methodology, Research and Scientific Method, Importance of Knowing How Research is Done, Research Process, Criteria of Good Research, Problems Encountered by Researchers in Ind

### Unit – II Survey of literature

Survey of literature including patents: Chemical nomenclature and literature-primary sources secondary sources including reviews, treatises, and monographs, -literature searching-review of work relevant to the chosen problems. Reviews: Annual and quarterly reviews, general reviews.

### Unit III - Computers and web-based research

Introduction, The Computer and Computer Technology, The Computer System, Important Characteristics Computer Applications Computers and Researcher,

Web sources for literature, Scifinder and other search engines Abbreviations used in scientific writing, ASAP Alerts, CA Alerts, Sci Finder, Chem Port, Science Direct, STN International. Google, scholar, Scopus-Journal home pages

### Unit - IV: Data Analysis

Data Analysis: Frequency distributions, the binomial distribution, the Poisson distribution and normal distribution – describing Data, population and sample, mean, variance, standard deviation.

Usage of data / graphical processing softwares (freeware)

Hypothesis testing, levels of confidence and significance, test for an outlier, testing variances, means t-Test, paired t-Test – Analysis – of variance (ANOVA) – Correlation and Regression – Curve fitting, Fitting of linear equations, simple linear cases. General polynomial fitting, linearizing transformations, exponential function fit – r and its abuse – Basic aspects of multiple linear regression analysis.

### **Unit** – **V** - Writing a scientific paper and thesis

Meaning of Interpretation, Why Interpretation, Technique of Interpretation: Precaution in Interpretation Significance of Report Writing Different Steps in Writing Report Layout of the Research Report Types of Reports Oral Presentation Mechanics of Writing a Research Report Precautions for Writing Research Reports

#### References

- 1. C.R Kothari, Research Methodology, New Age International publishers, 2<sup>nd</sup>Edn; 2009.
- 2. Goode, William J., and Natt, Paul K.Methods in social research, International Student edition, McGraw-Hill Co, and Kogakusha Ltd., 1995.
- 3. Bates, R.N and Schoofer, J.P., Research Techniques in Organic Chemistry, Prentice Hall
- 4. B. E. Cain, The Basis of Technical Communicating, ACS., Washington, D.C., 1988.
- 5. J. W.Best, Research in Education, 4th ed. Prentice Hall of India, New Delhi, 1981.
- 6. H. F. Ebel, C. Bliefert and W.E. Russey, The Art of Scientific Writing, VCH, Weinheim, 1988.
- 7. J. Gibaldi, and W.S. Achtert, Handbook for writers of Research Papers; 2nd ed.; Wiley Eastern, 1987.
- 8. Joseph, Methodology for Research; Theological Publications, Bangalore, 1986.
- 9. R. L. Dominoswki, Research Methods, Prentice Hall, 1981.
- H. M. Kanare, Writing the Laboratory Notebook; American Chemical Society: Washington, DC, 1985.

### Syllabus:

### **SEMESTER-II**

### HETEROCYCLIC CHEMISTRY

Course Code	CH821B		Credit	4
Instruction Hours per Week	4		Marks	CIA (50) / SE (50)
Course Objective	•	To learn the nature compounds To understand the heterocyclic compo	re and reaction classification unds.	ons of heterocyclic and significance of

#### **Course Outcomes**

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

CO. No.	Course Outcome Statement	Cognitive Level
CO 1	Acquire basic knowledge on classifications of Heterocyclic Compounds, nomenclature of Heterocyclic Compounds, structural characteristics, physical properties, synthesis of Heterocyclic Compounds and chemical reactions.	K1, K2
CO 2	Analyze and discuss the Information and data related to Heterocyclic Compounds.	K3, K4
CO 3	Detecting and leading the reactivity and stability of hetero aromatic compounds.	K5, K6
CO 4	Demonstrate the proficiency in designing reaction schemes to achieve six and seven membered ring heterocycles.	K6
CO 5	Apply these hetero aromatic compounds in the synthesis of important industrial and pharmaceutical compounds.	K5, K6
CO 6	Understand the chemistry of large heterocyclic structures and plan to synthesize them	K1, K6

## Mapping of CO with PO and PSO

Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)							
СО	PO 1	PO 2	PO 3	PO 4	PO 5	PSO 1	PSO 2	PSO 3	PSO 4	PSO 5	PSO 6	Mean Score s of COs
- CO 1	3	3	3	3	2	3	3	2	2	3	3	2.73
- CO 2	3	3	2	3	2	3	3	3	2	3	2	2.64
- CO 3	3	2	3	3	2	3	3	2	2	3	3	2.64
- CO 4	3	2	3	3	2	3	3	3	2	2	3	2.64
- CO 5	3	3	3	3	3	3	3	2	3	3	3	2.91
- CO 6	3	3	3	3	2	3	3	3	3	3	3	2.91
Mean Overall Score								2.74				
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: Nomenclature of Heterocycles**

Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic fused and bridged heterocycles. Aromatic Heterocycles General chemical behaviour of aromatic heterocycles, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in 1H NMR-spectra. Empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations). Heteroaromatic reactivity and tautomerism in aromatic heterocycles.

### Unit - II: Non-Aromatic Heterocycles

Strain-bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction. Stereo-electronic effects anomeric and related effects, Attractive interactions-hydrogen bonding and intermolecular nucleophilic, ectrophilic interactions. Heterocyclic Synthesis. Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions.

### **Unit - III: Small Ring Heterocycles**

Three-membered and four-membered heterocycles-synthesis and reactions of azirodines, oxiranes, thiranes, azetidines, oxetanes and thietanes.Benzo-Fused Five-Membered HeterocyclesSynthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes.

#### **Unit - IV: Meso-Ionic Heterocycles**

General classification, chemistry of some important meso-ionic heterocycles of type-A and B and their applications. Six-membered Heterocycles with one Heteroatom. Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium&thiopyrylium salts and phridones. Synthesis and reactions of quionlizinium and benzopyrylium salts, coumarins and chromones.

### **Unit - V: Higher Heterocycles**

Six membered Heterocycles with two or more Heteroatoms. Synthesis and reactions of diazones, triazines, tetrazines and thiazines. Seven-and Large-membered Heterocycles. Synthesis and reactions of azepines, oxepines, thiepines, diazepinesthiazepines, azocines, diazocines, dioxocines and dithiocines.

#### References

- 1. G. K. Chatwal, Organic Chemistry on Natural Products, Vol. 1, Himalaya Publishing House, Mumbai, 2009.
- 2. G. K. Chatwal, Organic Chemistry on Natural Products, Vol. 2, Himalaya Publishing House, Mumbai, 2009.
- 3. O. P. Agarwal, Chemistry of Organic Natural Products, Vol. 1, Goel Publishing House, Meerut, 1997.
- 4. O. P. Agarwal, Chemistry of Organic Natural Products, Vol. 2, Goel Publishing House, Meerut, 1997.
- 5. L. Finar, Organic Chemistry Vol-2, 5<sup>th</sup> ed., Pearson Education Asia, 1975.
- 6. T. L. Gilchrist, Heterocyclic Chemistry, Longman Press, 1989.
- 7. J. A. Joule and K. Mills, Heterocyclic Chemistry, 4<sup>th</sup> ed., John-Wiley, 2010.
- 8. Raj K Bansal Heterocyclic chemistry, fourth edition, New Age International Publishers, 2005.

### CH821C – BIO - ORGANIC CHEMISTRY

Course Code	Туре	Total Hours	Lecture	Tutorial	Practical
CH821C	Theory	75	65	10	0
		Course Name		Max Marks	Credits
		BIO – ORGAN CHEMISTRY	NIC	100	4

### **Objectives:**

- To enable the student to understand and appreciate the importance of biomolecules.
- To understand the techniques involved in the extraction and methods of determination of structure of natural products.
- To describe the structure and function of nucleic acids
- To learn the synthetic procedure of alkaloids and terpenoids and their applications.
- To synthesis the steroids compounds and interpret their biological role.
- To Illustrate the method of synthesis of flavonoids.

#### **Course Outcomes**

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

CO. No.	Course Outcome Statement	Cognitive Level
CO 1	Understand and know the importance of the biomolecules	K1, K2
CO 2	Apply the extraction techniques and elucidate the structure of natural products.	K3, K4
CO 3	Describe the structure and function of DNA and RNA and justify the denaturation of nucleic acid	K2, K5
CO 4	Synthesis a common alkaloid and terpenoids and know their importance	K5
CO 5	Design the synthetic route of steroids and interpret their functions in biological system	K3, K6
CO 6	Describe the general method of synthesis of anthocyanins and flavonoids.	K2

#### **Course Content**

#### **Unit - I: Carbohydrates**

Configuration and conformations of monosaccharides, anomeric effect, epimerization and mutarotation. Determination of ring size of monosaccharides. Synthesis, industrial and biological importance of glycosides, amino sugars, sucrose and maltose. Industrial and biological importance of cellulose, starch, glycogen, dextran, hemicellulose, pectin, agar-agar, cytosine, crysin. Glycolysis and its reversal; TCA cycle. Relation between glycolysis and respiration.

### **Unit - II: Proteins and Nucleic Acids**

Classification – properties - 3D structure of protein; Determination of C and N-terminal amino acid sequence – denaturation and renaturation of proteins. Separation and purification of proteins – dialysis – gel filtration - electrophoresis. Catabolism of amino acids: transamination, oxidative deamination, decarboxylation and urea cycle. Introduction, structure and synthesis of nucleosides and nucleotides, protecting groups for hydroxy group in sugar, amino group in the base and phosphate functions. Methods of formation of internucleotide bonds: Structure of RNA and DNA, Crick-Watson model. Solid phase synthesis of oligonucleotides. Role of nucleic acids in the biosynthesis of proteins.

#### **15 Hours**

**15 Hours** 

### Unit - III: Alkaloids and Terpenoids

General methods of structural elucidation of alkaloids. Structural elucidation of apaverine and cocaine; synthesis and functions of atropine, heptaphylline, morphine. General methods of determination of structure of terpenoids. Structural elucidation of cadinene, vitamin A, abietic acid; synthesis and functions of gibberelic acid, zingiberine and squalene

### **Unit - IV: Steroids**

Conformations of stereoids - molecular rearrangements (acid, base catalysed, and photochemical). Synthesis of steroids – ring forming reaction and control of ring junction stereochemistry. Synthesis and functions of cholesterol, androgens, oestrone, progesterone and cortisone.

#### Unit - V: Anthocyanins and flavonoids

General nature and structure of anthocyanins. General methods of synthesizing anthocyanidins. Structural elucidation of cyanidin chloride, pelargolidin chloride, Hirsutidin chloride. Flavones – flavonols – isoflavones. Biosynthesis of flavonoids.

#### References

- 1. T. K Lindhorst, Essentials of Carbohydrate Chemistry and Biochemistry, Wiley VCH, 2007.
- 2. G. K. Chatwal, Organic Chemistry on Natural Products, Vol. 1, Himalaya Publishing House, Mumbai, 2009.
- 3. G. K. Chatwal, Organic Chemistry on Natural Products, Vol. 2, Himalaya Publishing House, Mumbai, 2009.
- 4. O. P. Agarwal, Chemistry of Organic Natural Products, Vol. 1, Goel Publishing House, Meerut, 1997.
- 5. O. P. Agarwal, Chemistry of Organic Natural Products, Vol. 2, Goel Publishing House, Meerut, 1997.
- 6. L. Finar, Organic Chemistry Vol-2, 5<sup>th</sup> ed., Pearson Education Asia, 1975.
- 7. L. Finar, Organic Chemistry Vol-1, 6<sup>th</sup> ed., Pearson Education Asia, 2004.
- 8. Pelletier, Chemistry of alkaloids, Van Nostrand Rein

### Mapping of CO with PO and PSO

	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)						
СО	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	Mean Scores of COs
CO1	3	2	3	3	2	3	3	3	2	3	3	2.73
CO2	3	2	3	3	3	3	3	2	3	3	3	2.82
CO3	3	3	3	2	2	3	3	2	3	2	3	2.64
CO4	3	3	3	2	2	3	3	2	3	3	3	2.73
CO5	3	3	3	3	2	3	3	2	3	3	3	2.82
CO6	3	3	3	2	2	3	3	3	2	3	3	2.73
Mean Overall Score									2.74			
Result										High		

#### **Assessment Pattern**

#### 15 Hours

**15 Hours** 

**15 Hours** 

Bloom's Category	CA Tests (Marks Allotme	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

### PCH813 – Organic Chemistry Practicals I

<b>Course Code</b>	Туре	<b>Total Hours</b>	Lecture	Tutorial	Practical
PCH813	Practical	60	4	0	56
		Course Name		Max Marks	Credits
		ORGANIC	CHEMISTRY	100	4
		PRACTICALS	-I		

#### **Objectives:**

- To learn the separation of an organic compound from the mixture and identify them using various chemical tests.
- To enable the student to learn the methods of preparation for some organic compounds.

#### **Course Outcomes:**

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

S.No	Course outcome	Cognitive level
CO-1	Identify and relate the nature of the organic compound mixture given based on solubility and reactivity	(K1, K2)
CO-2	Demonstrate the systematic analysis and separation of organic compound mixture into individual components	(K4)
CO-3	Experimenting organic chemistry theoretical knowledge into laboratory tests with respect to addition, oxidation, substitution reactions and other reactions	(K3)
CO-4	Correlate functional group and corresponding derivatives formed during qualitative analysis in the laboratory	(K4)
CO-5	Implement synthetic approach with single stage preparations in laboratory using oxidation, reduction etc.	(K3)
CO-6	Build and reflect the synthetic ability to prepare and purify organic compounds from single stage reactions	(K5, K6)

### **Course Content**

- 1. Separation and identification of components in a two-component mixture and preparation of their derivatives.
- 2. Any Six preparations from the following:
  - o p-Nitrobenzoic acid from p-nitrotoluene
  - Anthroquinone from anthracene
  - o Benzhydrol from benzophenone
  - m-Nitroaniline from m-dinitrobenzene
  - o 1,2,3,4 Tetrahydrocarbazole from cyclohexanone
  - p-Chlorotoluene from p-toluidine
  - 2,3 Dimethylindole from phenyl hydrazine and 2 butanone
  - Methyl orange from sulphanilic acid
  - Diphenyl methane from benzyl chloride

### **Reference Books:**

- 1. Arthur I. Vogel, "A Textbook of Practical Organic Chemistry", ELBS, 1969.
- 2. N.S. Gnanapragasam and B. Ramamoorthy, "Organic Chemistry Lab Manual", S. Visvanathan Printers & Publishers, 2006.

### Mapping of CO with PO and PSO

	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)						
со	PO 1	PO 2	PO 3	PO 4	PO 5	PSO 1	PSO 2	PSO 3	PSO 4	PSO 5	PSO 6	Mean Score s of COs
- CO 1	3	3	2	3	2	3	2	3	3	3	2	2.6
- CO 2	3	3	3	3	1	3	2	3	3	3	2	2.6
- CO 3	2	3	3	3	1	2	3	2	3	3	2	2.5
- CO 4	3	3	2	2	1	3	2	2	3	2	2	2.3
- CO 5	3	3	2	3	1	3	3	3	2	3	3	2.6
- CO 6	3	3	2	2	1	2	2	2	3	3	2	2.3
Mean Overall Score										2.5		
Resu	lt											High

### Scheme of Valuation

### **External Component:**

60 Marks and it has to be converted to 50 Marks

S. No	Components	Mark Distribution
1	Qualitative analysis of Organic mixtures	30
2	Single stage organic compound preparation	15
3	Record	05
4	Viva	10
	Total Marks	60 Marks

### i) Qualitative Analysis of Organic compounds

Identification of TWO organic compounds in a given mixture

Pilot test report	= 4 Marks
Identification of TWO individual organic compounds (2×13 M)	= 26 Marks
Without procedure TWO components report (2*5 M)	= 10 marks

For each single organic compound, mark distribution as follows:

Components	Mark distribution
Aliphatic/ Aromatic	1 mark
Saturation/Unsaturation	1 mark
Special elements (N,S,X)	3 marks
Functional group	5 marks
Derivative	3 marks
Total	13 Marks

### ii) Single stage preparation:

Crude sample in single stage preparation = 10 Marks

Recrystallization

= 05 Marks

### **Internal Component:**

S. No	Components	Mark Distribution
1	Qualitative analysis of Organic Mixtures <sup>*</sup>	20
2	Single stage organic compound preparation	10
3	Viva <sup>‡</sup>	05
4	Theory of Practical's <sup>‡</sup>	05
5	Model practical examination	10
	Total Marks	50 Marks

#### **Conditions for Internal Component:**

For Component 1 to 3 60% of the work done has to take into account

ONE Viva and One TOP per semester has to be taken into account

\* In-case of Pandemic Outbreak an average practical's that is done has to be taken into consideration.

<sup>‡</sup> In-case of Pandemic Outbreak the best of Viva and Theory of Practical's conducted has to be taken for calculation in internal component.

### PCH814 - Inorganic Chemistry Practicals – I

Course Code	Туре	<b>Total Hours</b>	Lecture	Tutorial	Practical
PCH814	Practicals	60	4	0	56
		Course Name		Max Marks	Credits
		INORGANIC	CHEMISTRY	100	4
		PRACTICALS-	·I		

#### **Course Objectives:**

- To learn the basic principles of qualitative analysis of an inorganic mixture
- To understand and apply the principles of complexometric titrations.

#### **Course Outcomes**

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

S. NO	Course Outcomes Statement	Cognitive level
CO1	Understand the methodology of determining ions using complexometric titrations.	K1
CO2	Devise methods to prepare a complex from simple starting materials	К3
CO3	Employ a standard procedure to identify the common and rare ions	K4, K6
CO4	Demonstrate the ability to identify and separate any ions from any mixtures by evolving the procedure	К6
CO5	Analyse the data obtained through various experiments and deduce conceptual explanations for theoretical concepts	К5

### **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.

### Mapping of CO with PO and PSO

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

#### **Scheme of Valuation**

### **External Component:**

100 Marks and it has to be converted to 50 Marks

S. No	Components	Mark Distribution			
1	Quantitative analysis of Inorganic Mixtures	40	20		
2	Volumetric Analysis-Complexometric titration	20	10		
3	Preparation of Complexes	20	10		
4	Viva	10	05		
5	Record	10	05		
	Total Marks	100 Marks	50 M		

### i) Quantitative Analysis:

Detection of TWO Common radicals and TWO Uncommon Radicals

With complete procedure $(4 \times 10 \text{ M})$	= 40 Marks
Identification of radicals/Group (4×2 M)	= 08 Marks

#### ii) Volumetric Analysis:

#### Error Calculation

$\leq$ 2% Error	= 20 Marks
2-3 Error	= 20-15 Marks
3-4 Error	= 15-10 Marks
$\geq$ 4 Error	= 10 Marks

### ii) Complex Preparation:

Preparation of Complex	= 15 Marks
Quality and Quantity of the Complex Prepared	= 05 Marks

### **Internal Component:**

100 Marks and it has to be converted to 50 Marks

S. No	Components	Mark Distribution			
1	Quantitative analysis of Inorganic Mixtures <sup>*</sup>	40	20		
2	Volumetric Analysis-Complexometric titration*	20	10		
3	Preparation of Complexes <sup>*</sup>	20	10		
4	Viva <sup>‡</sup>	05	2.5		
5	Theory of Practical's <sup>‡</sup>	05	2.5		
6	Model Examination	10	05		
	Total Marks	100 Marks	50 M		

### **Conditions for Internal Component:**

For Component 1 to 3 60% of the work done has to take into account

ONE Viva and One TOP per semester has to be taken into account

\* In-case of Pandemic Outbreak an average practical's that is done has to be taken into consideration.

<sup>‡</sup> In-case of Pandemic Outbreak the best of Viva and Theory of Practical's conducted has to be taken for calculation in internal component.

### PCH815 – PHYSICAL CHEMISTRY PRACTICALS I

Course Code	Туре	<b>Total Hours</b>	Lecture	Tutorial	Practical
PCH815	Practicals	60	4	0	56
		Course Name		Max Marks	Credits
		PHYSICAL	CHEMISTRY	100	4
		PRACTICALS	-I		

**Objectives:** 

• To learn various physical and electrochemical methods to perform chemical measurements

### **Course Outcomes**

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

CO. No.	Course Outcome Statement	Cognitive Level
CO 1	Knowledge of measuring and determining the rate, order, rate constants of chemical reactions experimentally.	K1
CO 2	Understand and use the concept of distribution coefficient to measure the equilibrium constant.	K2
CO 3	Applying the concept of optical activity to measure the rate constant and to compare the strength of acids.	К3
CO 4	Experimenting the relation between the amount of molecule adsorbed on the surface of a adsorbent and apply the concepts of adsorption in the field of catalysis.	K3, K5
CO 5	Construct the phase diagram and apply it to metallurgical industry.	К3
CO 6	Estimate the minimum energy required for the molecules to undergo chemical reactions.	К4
CO 7	Evaluate the speed of chemical reactions in terms of temperature, concentration, and ionic strength.	K5
CO 8	Apply chemical kinetics in solving problems related to dosage and stability of drugs, absorption, distribution, and elimination of drugs from the body.	K3, K6
CO 9	Linking between the theoretical concepts with the experimental data obtained in the chemical kinetics.	K4

#### **Course Content**

Experiments in Thermodynamics, colligative properties, phase rule, chemical equilibrium and chemical kine Typical examples are given and a list of experiments is also provided from which suitable experiments can lessele as convenient.

- Heat of solution from Solubility measurements
- Determination of molecular weight
- Determination of activity and activity coefficient
- Phase diagram construction involving two/three component systems
- Determination of partial molar quantities
- Adsorption isotherm
- Reaction rate and evaluation of other kinetic parameters using polarimetry, analytical techniques, conductometry, dilatometry
- Verification of Beer Lambert law

Detailed list of Experiments for Physical Chemistry Practical I

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. Determine the temperature coefficient and energy activation of hydrolysis of ethyl acetate.
- 2. Study the kinetics of the reaction between acetone in iodine and acidic medium by half-life method and determine the order with respect to iodine and acetone.
- 3. Study the effect of solvent (DSMO-water, acetone-water system). On the rate of acid catalyzed hydrolysis of acetal by dilatometry.
- 4. Study the Saponification of ethyl acetate with sodium hydroxide by conductometrically and determine the order of the reaction.
- 5. Determine the order with respect to Silver (I) in the oxidation by spt and rate constant and for uncatalyzed reaction.
- 6. Study the inversion of cane sugar in the presence of acid using Polari meter.
- 7. Determine the rate constant and order of the reaction between potassium persulphate and potassium iodide and determine the temperature coefficient and energy of activation of the reaction.
- 8. Study the effect of ionic strength on the rate constant for the saponification of an ester.
- 9. Study the salt effect on the reaction between acetone and iodine.
- 10. Study the kinetics of the decomposition of sodium thiosulphate by mineral acid (0.5M HCI).
- 11. Study the primary salt effect on the kinetics of ionic reactions and test the Bronsted relationship (iodide ion is oxidized by persulphate ion).
- 12. Study the kinetics of enzyme catalysed reactions (Activity of tyrosinase upon tyrosine spectrophotometrically).
- 13. Study the salt effect, the solvent effect on the rate law of alkaline hydrolysis of crystal violet.
- 14. Study the reduction of aqueous solution of ferric chloride by stannous chloride.
- 15. Determine the molecular weight of benzoic acid in benzene and find the degree of association.
- 16. Determine the activity coefficient of an electrolyte by freeing point depression method.
- 17. Study the phase diagram form-toluidine and glycerine system.
- 18. Construct the phase diagram for a simple binary system naphthalene phenantherene and benzophenone-diphenyl amine.
- 19. Construct the boiling point composition diagram for a mixture having maximum boiling point and minimum boiling point.
- 20. Study the complex formation between copper sulphate and ammonia solution by partition method.
- 21. Study the simultaneous equilibria in benzoic acid benzene water system.
- 22. Determine the degree of hydrolysis and hydrolysis constant of aniline hydrochloride by partition method.
- 23. Determine the molecular weight of a polymer by viscosity method.
- 24. Determine the viscosities of mixtures of different compositions of liquids and find the composition of a given mixture.
- 25. Determine the partial molal volume of glycine/methanol/formic acid/sulphuric acid by graphical method and by determining the densities of the solutions of different compositions.

- 26. Study the temperature dependence of the solubility of a compound in two solvents having similar inter molecular interactions (benzoic acid in water and in DMSO water mixture) and calculate the partial molar heat of solution.
- 27. Determine the polar molar volume of glycine/methanol/formic acid /sulphuric acid by graphical method and by determining the densities of solutions of different concentrations.
- 28. Construct the phase diagram of the three component of partially immiscible liquid system (DMSOwater-benzene; acetone-chloroform -water; chloroform-acetic acid-water)
- 29. Construct the phase diagram of a ternary aqueous system of glucose -potassium chloride and water
- 30. Study the surface tension concentration relationship for solutions (Gibb's equation)
- 31. Study the absorption of acetic acid by charcoal (Freundlich isotherm)
- 32. Study the complex formation and find the formula of silver-ammonia complex by distribution method.
- 33. Determine the dissociation constant of picric acid using distribution law.

#### **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.

## Mapping of CO with PO and PSO

	Programme Outcomes (POs)					Programme Specific Outcomes (PSOs)						
СО	PO 1	PO 2	PO 3	PO 4	PO 5	PSO 1	PSO 2	PSO 3	PSO 4	PSO 5	PSO 6	Mean Score s of COs
- CO 1	3	3	2	3	2	3	1	3	3	3	1	2.45
- CO 2	3	3	2	3	2	3	1	3	3	3	1	2.45
- CO 3	3	3	3	3	2	3	2	3	3	2	1	2.55
- CO 4	3	3	3	2	3	3	1	3	3	3	1	2.55
- CO 5	3	3	3	3	3	3	2	3	3	3	1	2.73
- CO 6	3	3	2	3	2	3	2	3	3	2	1	2.45
CO 7	3	3	3	3	2	3	2	3	3	3	1	2.64
CO 8	3	3	3	3	2	3	3	3	3	3	3	2.91
CO 9	3	3	2	3	2	3	2	3	3	2	2	2.55
Mean	Overa	ll Score	e									2.59
Resul	ι											nign

### Scheme of Valuation

### **External Component (50 Marks):**

Component	Marks
Principle and procedure (Written)	05
Experiment	30
Record	10
Viva	05
Total	50 Marks

## Internal Component (50 Marks):

Component	Marks
Regular practical (Average of best 70% of the practicals)	30
Model exam	10
Theory of practical (At least one per semester)	05
Viva (At least one per semester)	05
Total	50 Marks

## Mark distributions for Experiment (30 marks)

## 1. Phase Study

Component			Marks
Determination	n of unkno	own composition	15
% of	Marks		
error			
≤10	15		
10 - 15	10		
>15	05		
Phase diagram	n		05
Eutectic temp	berature ar	nd composition	10
Total			30

## 2. Equilibrium constant

Component			Marks
Determination	n of unkno	wn concentration	15
% of error	Marks		
≤10	15		
10 - 15	10		

>15	05			
Determination	of equili	brium constant	05	
Determination	ı of Distri	bution coefficient	05	
Calculations			05	
Total			30	

### 3. Salt effect (Persulfate Vs Iodide)

Comp	onent		Marks
Determination	n of unkno	own concentration of salt	15
% of error	Marks		
≤10	15		
10 - 15	10		
>15	05		
Determination	n of rate c	onstant by graphical method	10
Calculations of	of ionic st	rength of salt	05
Total			30

### 4. Determination of order of reaction (Persulfate Vs Iodide)

Component			Marks
Determination of orde	er with re	espect to KI	15
(Or)	)		
Determination or ord	er with re	espect to K <sub>2</sub> S <sub>2</sub> O <sub>8</sub>	
% of error	Marks		
≤10	15		
10 - 15	10		
>15	05		

Determination of total order	05
Determination of Rate of reactions of each mixture (4x2.5)	10
Total	30

### 5. Determination of order of reaction (Reaction of Iodination of acetone)

Component		Marks
Determination of order with	respect to acetone	10
Result: Deviation from	1.0 to 1.1- 10 marks	
	1.1 – 1.5 – 08 marks	
	>1.5 - 05 marks	
Determination of order with	respect to Iodine	10
Result: Deviation from Zer	o up to 0.1- 10 marks	
	>0.1 - 05 marks	
Determination of rate consta	ant of each mixture by	05
graphical method		
Calculations		05
Total		30

### 6. Adsorption of acetic acid on charcoal:

Comp	onent		Marks
Determination	n of unkne	own concentration of acetic acid	15
% of error	Marks		
≤10	15		
10 - 15	10		
>15	05		
Graph			05
Calculations			10

Total	30
Total	30

Component		Marks 15	
Comparison of acid strength			
% of error	Marks		
≤10	15		
10 - 15	10		
>15	05		
Rate constant	determina	tion by graphical method	7.5
Rate constant	determina	tion by calculation	7.5
Total			30

## 7. Comparison of acid strengths by Polarimeter and Ester hydrolysis

### 8. Determination of Energy of Activation (Ester hydrolysis reaction)

Component			Marks
Determination of energy of activation			15
% of error	Marks		
≤10	15		
10 - 15	10		
>15	05		
Determination Rate constant at two different temperatures			10
for both graphical and calculation			
Determination of pre exponential factor			05
Total			30

