

2020

# **M.Sc. CHEMISTRY**

## **Course Structure and Syllabus**

(For the candidates admitted from the academic year 2020-2021 onwards)

# **CHOICE BASED CREDIT SYSTEM (CBCS)**



**THANTHAI HANS ROEVER COLLEGE (AUTONOMOUS)**

(Nationally Re-Accredited by NAAC with B<sup>++</sup>)

(Affiliated to Bharathidasan University, Tiruchirappalli)

**ELAMBALUR, PERAMBALUR – 621 220**



**Thanthai Hans Roever College (Autonomous), Elambalur, Perambalur - 621 220**

**M.Sc., CHEMISTRY- Course Structure Under CBCS**

(For the candidates admitted from the academic year 2020-2021 onwards)

Semester	Course Code	Title of the Course	Ins. Hours/ Weeks	Credits	Exam Hours	CIA (Max)	ESE (Max)	Total (Max)
1	20PCH1CC1	Aromaticity, Stereochemistry and Reaction Mechanism	6	5	3	25	75	100
1	20PCH1CC2	Chemistry of Lanthanides, Boranes, Coordination and Radioactivity	6	5	3	25	75	100
1	20PCH1CC3	Group theory, Quantum mechanics, Thermodynamic and Photochemistry	6	5	3	25	75	100
1	20PCH1CP1	Organic Preparations and Mixture Analysis	6	4	6	40	60	100
1	20PCH1CP2	Inorganic Qualitative Analysis and Colorimetric Estimations	6	4	6	40	60	100
<b>Total</b>			<b>30</b>	<b>23</b>	-	-	-	<b>500</b>
2	20PCH2CC4	Bio-Inorganic and Organometallics	6	5	3	25	75	100
2	20PCH2CC5	Spectroscopy of Organic Molecules	6	5	3	25	75	100
2	20PCH2EC1:1 20PCH2EC1:2 20PCH2EC1:3	(A) Concept and Modern in Chemistry/ (B) Metallo proteins, Enzymes and Natural products (*)/ (C) Supramolecular Chemistry	6	4	3	25	75	100
2	20PCH2CP3	Organic Estimation and Double stage preparations – Practical	6	4	6	40	60	100
2	20PCH2CP4	Inorganic Estimation and Complex Preparations – Practical	6	4	6	40	60	100
<b>Total</b>			<b>30</b>	<b>22</b>	-	-	-	<b>500</b>
3	20PCH3CC6	Photochemistry, Pericyclic reactions, Heterocycles and Reagents	6	5	3	25	75	100
3	20PCH3CC7	Spectroscopy of coordination complexes	6	5	3	25	75	100
3	20PCH3EC2:1 20PCH3EC2:2 20PCH3EC2:3	(A) Crystal structure, Organic solid state and Optical properties (*) (B) Selected topics in Chemistry (C) Agricultural Chemistry	6	4	3	25	75	100
3	20PCH3EC3:1 20PCH3EC3:2 20PCH3EC3:3	(A) Electro Organic Chemistry (B) Analytical Chemistry (*) (C) Medicinal Chemistry	6	4	3	25	75	100
3	20PCH3CP5	Physical Chemistry Non-Electrical Practical	6	4	6	40	60	100
<b>Total</b>			<b>30</b>	<b>22</b>	-	-	-	<b>500</b>
4	20PCH4CC8	Electrochemistry, Surface Phenomena and Statistical Thermodynamics	6	5	3	25	75	100

4	20PCH4EC4:1 20PCH4EC4:2 20PCH4EC4:3	(A) Instrumentation Techniques (B) Nano and Green Chemistry (*) (C) Inorganic and Organic Photochemistry	6	4	3	25	75	100
4	20PCH4EC5:1 20PCH4EC5:2 20PCH4EC5:3	(A) Industrial Chemistry (*) (B) Polymer Chemistry (C) Chemistry of Natural Products	6	4	3	25	75	100
4	20PCH4CP6	Physical Chemistry Electrical Practical	6	4	6	40	60	100
4	20PCH4PW	Project	6	6	-	-	-	100
<b>Total</b>			<b>30</b>	<b>23</b>	-	-	-	<b>500</b>
<b>Grand Total</b>			<b>120</b>	<b>90</b>	-	-	-	<b>2000</b>

CIA: Continuous Internal Assessment; ESE: End Semester Examination; CC: Core Course; EC: Elective Course.

#### List of Elective Courses

Elective	Course Code	Title of the Course
Elective -1	20PCH2EC1:1 20PCH2EC1:2 20PCH2EC1:3	(A) Concept and Modern in Chemistry (B) Metallo proteins, enzymes and Natural products (*) (C) Supramolecular Chemistry
Elective -2	20PCH3EC2:1 20PCH3EC2:2 20PCH3EC2:3	(A) Crystal structure, Organic solid state and Optical properties(*) (B) Selected topics in Chemistry (C) Agricultural Chemistry
Elective -3	20PCH3EC3:1 20PCH3EC3:2 20PCH3EC3:3	(A) Electro Organic Chemistry (B) Analytical Chemistry (*) (C) Medicinal Chemistry
Elective -4	20PCH4EC4:1 20PCH4EC4:2 20PCH4EC4:3	(A) Instrumentation Techniques (B) Nano and Green Chemistry (*) (C) Inorganic and Organic Photochemistry
Elective -5	20PCH4EC5:1 20PCH4EC5:2 20PCH4EC5:3	(A) Industrial Chemistry(*) (B) Polymer Chemistry (C) Chemistry of Natural products

**Note:**

Project : 100 Marks  
Dissertation : 80 Marks  
Viva Voce : 20 Marks

Core Papers - 8  
Core Practical - 6  
Elective Papers - 5  
Project - 1

1. Theory Internal 25 marks External 75 marks
2. Practical " 40 marks " 60 marks
3. Separate passing minimum is prescribed for Internal and External
  - a) The passing minimum for CIA shall be 40% out of 25 marks (i.e. 10 marks)
  - b) The passing minimum for Semester Examinations shall be 40% out of 75 marks (i.e. 30 marks)
  - c) The passing minimum not less than 50% in the aggregate.

## SEMESTER-I

Course Code: 20PCH1CC1  
Instruction Hours:6  
Credits: 5

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### CORE COURSE 1– AROMATICITY, STEREOCHEMISTRY AND REACTION MECHANISM

#### Course Outcomes:

- To enable the students to understand the concept of aromaticity
- To enable the students to understand basic stereochemistry concept in proper perspective.
- To enable the students to understand the concept of asymmetric synthesis.
- To enable the students to understand various types of reaction mechanisms involved in synthetic organic transformation.
- To enable the students to understand various types of nucleophilic substitution reaction.

#### Unit I

**Aromaticity:** Aromaticity – definition – Huckel’s and Craig’s rules – effects of aromaticity on bond lengths – ring currents – aromatic character in 3,4,5,6,7,8 member rings and non-benzenoid- rings with 2, 4, 8, 10, 14 and 18  $\pi$  electron systems. Concept of Homoaromaticity- Antiaromaticity –alternant and non-alternant hydrocarbons. Aromaticity of annulenes – 10, 12, 14, 16 and 18 annulenes, heteroannulenes, sydnones and fullerenes.

#### Unit II

**Stereochemistry:** Optical activity and chirality, Classification of chiral molecules as asymmetric and dissymmetric. Calculation of number of optical isomers. A brief Study of dissymmetry of allenes, biphenyls, spiro compounds, trans cyclooctane and cyclononene and molecules with helical structures absolute configuration - R, S notation of biphenyls and allenes. Stereochemistry of mono and di-substituted cyclopropane, cyclobutane, cyclopentane and cyclohexane. Zig-Zag representation of glucose. Fischer projection. Inter conversion of Sawhorse, Newmann and Fischer projections. Molecules with more than one asymmetric center (restricted to five carbons). e.g. Erythro and threo compounds.

#### Unit III

**Conformational Analysis:** Conformational analysis of disubstituted cyclohexane and their stereochemical features (geometric and optical isomerism (if shown) by these derivatives). Conformation and reactivity of substituted cyclohexanol (oxidation), cyclohexanone (reduction) and cyclohexane carboxylic acid derivatives (esterification and hydrolysis). Conformation and stereochemistry of cis and trans decalin and 9 - methyldecalin. Baeyer’s strain theory – alpha haloketone effect, 3-alkyl ketone effect, 2-alkyl ketone effect.

## UnitIV

**Aliphatic Nucleophilic Substitution Reaction:**  $SN^1$ ,  $SN^2$  and  $SN^i$  mechanisms - Neighboring group participation - reactivity, structural and solvent effects - substitution in norbornyl and bridgehead systems - substitution at allylic and vinylic carbons - substitution by ambident nucleophiles - substitution at carbon doubly bonded to oxygen and nitrogen - alkylation and acylation of amines, halogen exchange, Von-Braun reaction, alkylation and acylation of active methylene carbon compounds, hydrolysis of esters, Claisen and Dieckmann condensation. Role of LDA, crown ethers and phase transfer catalysts (PTC) in nucleophilic substitution reactions. Migration of double bond, keto-enol interconversion, HVZ reaction, Stark-Enamine reaction, halogenation of aldehydes and ketones and decarboxylation of aliphatic acids.

## UnitV

**Aromatic Electrophilic and Nucleophilic Substitution Reactions:** The arenium ion mechanism. Orientation and reactivity (ortho, meta and para directing groups). Typical reactions - nitration, halogenation, alkylation, acylation and diazonium coupling, Formylation, Reimer - Tieman reaction, Vilsmeier - Haack, Gattermann, Gattermann - Koch, Kolbe reaction. Synthesis of di- and tri-substituted benzenes from benzene or mono-substituted benzenes.

Aromatic nucleophilic substitution in aryl halides by Meisenheimer complex mechanism and benzyne mechanism. Reactions of aryl diazonium salts. Zeigler alkylation, Vicarious Nucleophilic Substitution (VNS), Chichibabin and Schiemann reactions

### Text Book(s):

1. Mukherji S.M. and S.P.Singh, Organic Reaction Mechanism, MacMillan India Ltd., 2010.(Unit-1)
2. Nasipuri. D., Stereochemistry of organic compounds, Principles and applications 2012. (Unit-2 & Unit-3)
3. Bansal R.K., Organic Reaction Mechanism, Mchill publication, 2015. ( Unit-3)
4. Aluwalya, Reaction Mechanism 5<sup>th</sup> Edition, Mchill publication, 2015. ( Unit-4 & Unit-5)
5. M.K. Jain, S. C. Sharma, Modern Organic Chemistry, Vishal Publishing Company, 2014. (Unit-5)

### Reference Book(s):

1. Organic Synthesis by R.O.C. Norman, Chapman and Hall, NY, 1980
2. Physical Organic Chemistry by Niel Isaacs, ELBS Publications 1987
3. Advanced Organic Chemistry, Part A and B, by Francis A. Carey and Richard J. Sundberg, 3rd Edition (1990), Plenum Press.
4. Advanced organic reaction mechanism and structure by J. March, Tata McGraw Hill.
5. Organic Chemistry, Graham Solomons, Stereochemistry, Conformation analysis and Mechanism by P.S. Kalsi, 2nd Edition (1993), Wiley Eastern Limited, Chennai.
6. Stereochemistry of carbon compounds by Ernest Eliel, 1993
7. Stereochemistry and Mechanism through solved problems by P.S. Kalsi. Wiley Eastern Ltd., (1994).

### Question Pattern

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
<b>I</b>	20PCH1CC1	Aromaticity, Stereochemistry and Reaction Mechanism	6	5						
<b>Course Outcomes (COs)</b>	<b>Programme Outcomes(POs)      Programme Specific Outcomes(PSOs)</b>									
	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PSO1</b>	<b>PSO2</b>	<b>PSO3</b>	<b>PSO4</b>	<b>PSO5</b>
<b>CO1</b>	✓		✓	✓	✓		✓	✓	✓	✓
<b>CO2</b>	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
<b>CO3</b>	✓		✓		✓	✓	✓	✓	✓	✓
<b>CO4</b>	✓		✓		✓	✓	✓	✓		✓
<b>CO5</b>	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42    Relationship: High										

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER-I

Course Code: 20PCH1CC2  
Instruction Hours: 6  
Credits: 5

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### CORE COURSE 2– CHEMISTRY OF LANTHANIDES, BORONES, COORDINATION AND RADIOACTIVITY

#### Course Outcomes:

- Learn the properties of lanthanides
- To appreciate the structure of boranes, carboranes, metal clusters and inorganic polymers.
- Distortion in co-ordination complexes concept of sigma and pi bonding in complexes.
- Application of substitution reactions in the synthesis of Platinum and Cobalt complexes.
- Learn the fusion and fission reactions of inorganic elements.

#### Unit I

**Chemistry of Lanthanides:** Studies and Application of Lanthanides and Actinides: Spectral and Magnetic properties- Methods of separation of Lanthanides and Actinides using complex formation, Solvent extraction, ion exchange, fractional crystallization. Organometallic Compounds of lanthanides, Application of lanthanides and actinides compounds in Industries, Use of lanthanides compounds as Shift reagents.

#### Unit II

**Boron Compounds and Clusters:** Chemistry of boron – borane, higher boranes, carboranes, borazines and boron nitrides, Classification, Nomenclature, preparation, Structure and Bonding, STYX numbers, Wade's rule. Carboranes- Types such as nido-closo, arachno-preparation properties and Structure. Metallocarboranes-a general study. Metal clusters: Chemistry of low molecularity metal clusters only, Structure of  $\text{Re}_2\text{Cl}_8$ ; multiple metal-metal bonds.

#### Unit III

**Coordination Chemistry: Theories of Metal-Ligand Bond:** VB theory and its limitations – Crystal field theory - splitting of d-orbitals under various geometries – Factors affecting splitting – CFSE and evidences for CFSE (Structural and thermodynamic effects) – Spectrochemical series – Jahn-Teller distortion – Spectral and magnetic properties of complexes – Site preferences - Limitations of CFT – Ligand field theory – MO theory – sigma – and pi-bonding in octahedral, square planar and tetrahedral complexes– Nephelauxetic effect – The angular overlap model.



#### **Unit IV**

**Coordination Chemistry: Reaction Mechanism:** Kinetics and mechanism of reactions in solution – labile and inert complexes – Ligand displacement reactions in octahedral and square planar complexes – acid hydrolysis, base hydrolysis and anation reactions – trans effect – theory and applications. Electron transfer reactions – electron exchange reactions – complementary and non-complementary types – inner sphere and outer sphere processes – Cross reactions and Marcus Hush theory - isomerisation and racemisation reactions of complexes – Molecular rearrangement – Reactions of four and six-coordinate complexes – Inter conversion between stereoisomers. Application of trans effect – synthesis of isomers of  $\text{Pt(II)}$  complexes – theories of trans effect and cis-trans isomerisation reaction. Application of substitution reactions in the synthesis of Platinum and Cobalt complexes.

#### **Unit V**

**Nuclear and Radiation Chemistry:** Properties of nucleus – different types of nuclear forces, Nuclear structure and nuclear stability, Nuclear models – liquid drop model, shell model of nucleus, Radioactivity and nuclear reactions, nuclear reactions induced by charged particles –  $Q$  value – nuclear reaction cross section, significance and determination – theory of nuclear fission, nuclear fusion, stellar energy. Hot atom chemistry, Nuclear fission and fusion reactors. The interaction of nuclear radiations with matter. Radiation hazards and therapeutics. Detectors and their principles. Tracer Application of radioisotopes in agriculture, industry and medicine. Isotope dilution and radio-activation methods of analysis.

#### **Text Book(s):**

1. J. D. Lee – “A New Concise Inorganic Chemistry”, 5th Edition, Oxford University Press, 2011. (Unit-1).
2. Wahid Malik, G. D. Tuli and R. D. Madan, “Selected Topic in Inorganic Chemistry”, S.Chand & Co., Ltd (2011). (Unit-2).
3. R.Gopalan, V.Ramalingam “Concise Coordination Chemistry”, Vikas Publishing House Pvt. Ltd., New Delhi, 2001. (Unit-3 & Unit-4)
4. H.J. Arnikaar “Essential of Nuclear Chemistry”, 4th Edition, New Age International, Publishers, 2011. (Unit-5).

#### **Reference Book(s):**

1. M.C. Day, J. Selbin, Theoretical Inorganic Chemistry, 2<sup>nd</sup> Ed., East West Press, 1985.
2. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 4<sup>th</sup> Ed., John Wiley & Sons, 198.
3. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic chemistry-Principles on structure and reactivity, 4<sup>th</sup> Ed, Pearson- education, (2002).
4. S.F.A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach, Oxford University Press, 1996.
5. D.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models in Inorganic Chemistry, 3<sup>rd</sup> Ed. 1994.
6. J.D. Lee, Concise Inorganic Chemistry, 5<sup>th</sup> Ed, Wiley, 1999.

7. D.F. Shriver, P.W. Atkins, Inorganic Chemistry, 3<sup>rd</sup> Ed, 1999.

### Question Pattern

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
<b>I</b>	20PCH1CC2	Chemistry of Lanthanides, Boranes, Coordination and Radioactivity	6	5						
<b>Course Outcomes (COs)</b>	<b>Programme Outcomes(POs)</b>					<b>Programme Specific Outcomes(PSOs)</b>				
	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PSO1</b>	<b>PSO2</b>	<b>PSO3</b>	<b>PSO4</b>	<b>PSO5</b>
<b>CO1</b>	✓		✓	✓	✓		✓	✓	✓	✓
<b>CO2</b>	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
<b>CO3</b>	✓		✓		✓	✓	✓	✓	✓	✓
<b>CO4</b>	✓		✓		✓	✓	✓	✓		✓
<b>CO5</b>	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER - I

Course Code: 20PCH1CC3  
Instruction Hours:6  
Credits: 5

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### CORE COURSE 3–GROUP THEORY, QUANTUM MECHANICS, DYNAMIC AND PHOTOCHEMISTRY

#### Course Outcomes:

- Understand the rules and concepts of group theory
- Learn the principles and postulates of quantum mechanics of simple systems.
- To understand and explore the reaction kinetics of fast reactions
- Know the limitations of classical thermodynamics in the evaluation of macroscopic properties and principles of activity and fugacity.
- Understand concepts photochemical reactions and radiation absorption and emissions involved reactions.

#### Unit I

**Elements of Group Theory:** Introduction – Symmetry elements, Symmetry operations, n-fold Proper axis of symmetry, Centre of Symmetry, Plane of Symmetry, n-fold Improper axis of Symmetry, Group, Rules for forming a Group, Finite Group, Infinite Group, Abelian Group, Cyclic Group, Sub Groups, Group Multiplication Table- Class and Similarity transformation. Point Group – Method of Assigning Point Group, Matrix Representation Theory – Matrix Representation of Symmetry operation, Reducible, Irreducible Representation The Great Orthogonality Theorem – Properties of Irreducible Representation – Construction of Character Table for  $C_{3V}$ ,  $C_{2V}$  Point Groups – Explanation of Character Table – Correlation Table.

#### Unit II

**Basic concept of classical and quantum mechanical:** Classical mechanics – General principles, basic assumptions, postulates of classical mechanics, conservation laws, Lagrange and Hamilton equations of motion (no derivation). Operator algebra: operator, linear and hermitian, eigen functions and eigen values, angular momentum operator, commutation relations. Application of wave mechanics to simple systems - particle in a box, one- and three-dimensional - distortion of the box and Jahn-Teller effect - quantum numbers. Orthogonalisation and normalization – Potential barrier of definite thickness: Quantum mechanical tunneling.

#### Unit III

**Chemical Kinetics:** Theories of reaction rate - Absolute reaction rate theory (ARRT) - significance of reaction coordinate - Potential energy surfaces - Kinetic isotopic effect - molecular dynamics - Marcus theory of electron transfer processes - Principle of microscopic reversibility - Steady-state approximation. Chain reactions - thermal and photochemical reactions between hydrogen and bromine - explosions and hydrogen –

oxygen reactions. Factors influencing reaction rates in solution - application of ARRT to solution kinetics - effect of solvent and ionic strength, influence of pressure on rates in solution - significance of volume of activation

#### **Unit IV**

**Classical Thermodynamics:** Thermodynamics of systems of variable composition - partial molar property – partial molar quantities of E, V, H, A, G and S, chemical potential, physical significance of chemical potential, variation of chemical potential with respect to T and P, chemical potential in terms of U and H, partial molar quantities from experimental data – direct method, apparent molar properties, intercepts method and general methods. Calculation of thermodynamic properties of real gases - fugacity concept, variation of fugacity with T and P – calculation of fugacity of real gases, determination of fugacity – graphical method, equation of state method, determination of fugacity in gas mixtures –Lewis-Randall rule.

#### **Unit V**

**Photochemistry and Radiation Chemistry:** Photochemistry and Radiation chemistry: Photo physical process in electronically excited molecules - Jablonski diagram - Primary and Secondary Processes, quantum yield and its determination – Excimers and exciplexes- Kinetics of collisional quenching- Stern-Volmer equation - Chemical Actinometers - Photosensitization, Chemiluminescence. Photosynthesis, solar energy conversions. Semiconductor photo catalysis-Lasers and their applications.

Radiation chemistry:- Sources of high energy radiation - radiolysis of water – solvated electrons - Scavenging techniques - Applications of radiation chemistry.

#### **Text Book(s):**

1. K.V.Raman Group theory and its Application to Chemistry. Tata McGraw –Hill Publishing Company Limited New Delhi,2000.(Unit-1)
2. R.K.Prasad, Quantum Chemistry, New Delhi, Wiley-Eastern Ltd, 1992. (Unit-2)
3. K. J. Laidler, Chemical Kinetics,2nd ed, Tata McGraw Hill (1975). (Unit-3).
4. J.Rajaram and J. C. Kuriacose, Thermodynamics for Students of Chemistry, Lal Nagin Chand, New Delhi, (1986). (Unit-4).
5. K. K. Rohatgi and Mukerjee, Fundamentals of Photo Chemistry, Wiley Eastern Ltd (1986) (Unit-5)
6. G. Hughes, Radiation Chemistry, Oxford University Press(1973). (Unit-5)

#### **Reference Book(s):**

1. F.A.Cotton, Chemical Application of Group Theory. 2<sup>nd</sup> Edn. Wiley – Eastern Press,1995.
2. K. Veera Reddy, “Symmetry and Spectroscopy of Molecules”, New Age International Publishers, 2010.
3. A.K.Chandra, “Introductory Quantum Chemistry” 4th edition; Tata – McGraw Hill, 2010.
4. F.L.Pillar, Elementary Quantum Chemistry, McGraw Hill, 1970
5. Frost and R. G. Pearson, Kinetics and Mechanisms, John Wiley & Sons (1953).

6. J. C. Kuriacose and J. Rajaram, Kinetics and Mechanisms Transformations, Macmillan & Co., (1993).
7. Paula, Peter Atkins and Juliode, Elements of Physical Chemistry, 5th Ed, Oxford U.P, (2012).
8. Kloz and P. M. Rosenberg, Chemical Thermodynamics: Basics Theory and Methods, 3<sup>rd</sup> Ed., W. A. Benjamin, NY (1974).
9. R. P. Rastogi and R. R. Misra, An Introduction to Chemical Thermodynamics, Vikas Publishing House Pvt Ltd., (1992)
10. S. Glasstone, Thermodynamics for Chemists, East-west Affiliated Pvt Ltd, New Delhi (1969).
11. N. J. Turro, Modern molecular photochemistry, Benjamin/Cummings, Menlo Park, California, 1978.

### Question Pattern

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
<b>I</b>	20PCH1CC3	Group Theory, Quantum Mechanics, Dynamic and Photochemistry	6	5						
<b>Course Outcomes (COs)</b>	<b>Programme Outcomes(POs)</b>					<b>Programme Specific Outcomes(PSOs)</b>				
	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PSO1</b>	<b>PSO2</b>	<b>PSO3</b>	<b>PSO4</b>	<b>PSO5</b>
<b>CO1</b>	✓		✓	✓	✓		✓	✓	✓	✓
<b>CO2</b>	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
<b>CO3</b>	✓		✓		✓	✓	✓	✓	✓	✓
<b>CO4</b>	✓		✓		✓	✓	✓	✓		✓
<b>CO5</b>	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER - I

Course Code: 20PCH2CP1  
Instruction Hours: 6  
Credits: 4

Exam Hours: 6  
Internal Marks: 40  
External Marks: 60

### CORE COURSE PRACTICAL 1 – ORGANIC PREPARATIONS AND MIXTURE ANALYSIS - PRACTICAL

#### Course Outcomes:

- To enable the students to learn about separation technique of organic compounds.
- Be able to learn qualitative analysis of organic compounds.
- Synthesize the students to understand simple double stage preparations of some organic complex.
- To enable the students to learn about find out melting point of organic compounds.
- To enable the students to learn about preparations of derivatives.

#### 1. Separation of Organic Mixtures

- I. Pilot separation
- II. Bulk separation
- III. Determination of melting point/boiling point
- IV. Analysis of Soluble/Insoluble component:
  - a) Aliphatic/Aromatic
  - b) Saturation / Unsaturation
  - c) Special elements
  - d) Functional group
  - e) Derivatives

#### 2. Preparations – (Two stages)

- I. Acetanilide to *p*-bromoacetanilide to *p*-bromoaniline.
- II. Acetanilide to *p*-nitroacetanilide to *p*-nitroaniline.
- III. Preparation of  $\text{Cu}_2\text{Cl}_2$ ; 2-chlorobenzoic acid from anthranilic acid.
- IV. Benzoin to benzil to benzilic acid.

#### Reference Book(s):

1. A.I. Vogel, A.R. Tatchell, B.S. Furniss, A.J. Hannaford, P.W.G. Smith, Vogel's Textbook of Practical Organic Chemistry, 5<sup>th</sup> Ed., Prentice Hall, 1996.
2. J. Mohan, Organic Analytical Chemistry, Theory and Practice, Narosa, 2003.
3. V.K. Ahluwalia, P. Bhagat, R. Aggarwal, Laboratory Techniques in Organic Chemistry, I.K. International, 2005.

4. N.S. Gnanaprakasam, G. Ramamurthy, Organic Chemistry Lab Manual, S.V. Printers, 1987.

#### Scheme of valuation

Criteria	Marks	
<b>Record</b>	5	
<b>Procedure writing</b>	10	
<b>Organic preparation</b>	15	
<b>Analysis</b>		
	<b>I</b>	<b>II</b>
<b>Aliphatic/aromatic</b>	2	2
<b>Saturated/unsaturated</b>	2	2
<b>Element test</b>	4	4
<b>Functional group</b>	5	5
<b>Derivative</b>	2	2

#### Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
<b>I</b>	20PCH2CP1	Organic preparations and mixture analysis - practical	6	4						
<b>Course Outcomes (COs)</b>	<b>Programme Outcomes(POs)</b>					<b>Programme Specific Outcomes(PSOs)</b>				
	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PSO1</b>	<b>PSO2</b>	<b>PSO3</b>	<b>PSO4</b>	<b>PSO5</b>
<b>CO1</b>	✓		✓	✓	✓		✓	✓	✓	✓
<b>CO2</b>	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
<b>CO3</b>	✓		✓		✓	✓	✓	✓	✓	✓
<b>CO4</b>	✓		✓		✓	✓	✓			✓
<b>CO5</b>	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER - I

Course Code: 20PCH2CP2  
Instruction Hours: 6  
Credits: 4

Exam Hours: 6  
Internal Marks: 40  
External Marks: 60

### CORE COURSE PRACTICAL 2 – INORGANIC QUALITATIVE ANALYSIS AND COLORIMETRIC ESTIMATIONS - PRACTICAL

#### Course Outcomes:

- To enable the students to learn about inorganic qualitative analysis.
- Be able to learn quantitative separation of metal ions in binary mixtures.
- To enable the students to learn knowledge about analysis of rare earth elements.
- Use colorimeter to estimate inorganic compounds.
- Synthesize the students to understand simple single stage preparations of some inorganic complex.

#### 1. Semi-micro Qualitative Analysis

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

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

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

#### 2. Colorimetric Estimation:

Cu, Fe, Mn, Ni, Cr

#### Reference Book(s):

- 1.V.V. Ramanujam, Inorganic Semi Micro Qualitative analysis, National Pubs, 1988.
- 2.A.I. Vogel, Text Book of Quantitative Inorganic Analysis, 3<sup>rd</sup> Ed., Longman, 1966.

#### Scheme of Valuation

Criteria	Marks		
Record	5		
Aim and tabulation	5		
Mixture analysis [30]		Colorimetry [20]	
4- radicals with correct procedure	30	Error	Marks
3- radicals with correct procedure	25	< 1 %	20
2- radicals with correct procedure	20	1-2%	15
1- radical with correct procedure	10	2-3%	
Spotting	10	3%	10
			5



Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course					Hours	Credits			
I	20PCH2CP2	Inorganic qualitative analysis and colorimetric estimations - practical					6	4			
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)					
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	
CO1	✓		✓	✓	✓		✓	✓	✓	✓	
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
CO3	✓		✓		✓	✓	✓	✓	✓	✓	
CO4	✓		✓		✓	✓	✓	✓		✓	
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓	
Number of Matches(✓) = 42 Relationship: High											

Mapping	1-29%	30-59%	60-69%	70-89%	90-100%
Matches	1-14	15-29	30-34	35-44	45-50
Relationship	Very Poor	Poor	Moderate	High	Very High

## SEMESTER - II

Course Code: 20PCH1CC4  
Instruction Hours: 6  
Credits: 5

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### CORE COURSE 4– BIO-INORGANIC AND ORGANOMETALLICS

#### Course Outcomes:

- To enable the students to understand the importance of transport and storage metals in biological systems.
- To enable the students to understand the importance of Fe, Mg and Cu-containing proteins.
- To enable the students to understand the structure and importance of biomolecules of proteins and metal in proteins
- To enable the students to understand the importance of trace elements in biological system and also the toxicity of metal ions and understand the role of metals in medicine.
- To enable the students to learn the various types of reactions of coordinated ligands in organometallics.

#### Unit I

**General Principles of Bioinorganic Chemistry:** Occurrence and availability of Inorganic elements in Organisms - Biological function of inorganic elements - Biological ligands for metal ion coordination of proteins and enzymatic catalysis – Porphyrins and other Macrocycles – Nucleobases, nucleotides and Nucleic acids as ligands, bleomycin and siderophores- Communication roles for metals in biology.

**Transport and storage of metals:** Mechanism Fe, Cu, Zn and V storage and transport – metallothioneins. Molecular mechanism of iron transport across the membrane – sodium and potassium ion pumps. Metals at the Center of Photosynthesis: Primary Processes in Photosynthesis – Photosystems I and II.

#### Unit II

**Oxygen Transport and energy transfer of metals proteins:** Reactions of the alkyl cobalamins – One-electron Reduction and Oxidation – coenzyme B<sub>12</sub> – Alkylation reactions of methylcobalamin. Heme and Non-heme Proteins: Hemoglobin and Myoglobin – Hemerythrin - Oxygen transport and storage – Electron transfer - Ferredoxins and Rubredoxins – Cytochromes – Cytochrome C Oxidase - Oxygen activation – Mononuclear non-heme iron enzymes model systems.

**Copper containing proteins:** Classification – blue copper proteins – structure of blue copper electron transferases – copper protein as oxidases.

#### Unit III

**Medicinal Bioinorganic Chemistry:** Bioinorganic Chemistry of quintessentially toxic metals. Lead, Cadmium, Mercury, Aluminum, Chromium, Iron, Copper, Plutonium.

Chemotherapy: Chemotherapy with compounds of certain non-essential elements. Platinum complexes in Cancer therapy – Cisplatin and its mode of action – Cytotoxic compounds of other metals – Gold containing drugs as anti-rheumatic agents and their mode of action - Lithium in Psychopharmacological drugs.

#### **Unit IV**

**Organometallics: Basic Concepts:** Types of organometallic compounds on the basis of the nature of M-C bond. EAN rule: 18e- and 16e- rules – determinant of oxidation state, configuration, coordination number of the metal centre – Types and application 18e<sup>-</sup> / 16e<sup>-</sup> rules. Preparation, properties, structure and bonding in Metal carbonyls, nitrosyls, Metal olefins, acetylenes, Metallocene and arene complexes.

– fluxional organometallic compounds – application of organometallics.

#### **Unit V**

**Organometallic Chemistry:** Reactions and Catalysis by Organometallics: Organometallic reactions – Ligand association and dissociation – carbonylation and decarbonylation; oxidative addition and reductive elimination, insertion and deinsertion (elimination). Template synthesis of macrocyclic ligands.

Reactions of coordinated ligands in organometallics - Hydrogenation, hydroformylation, epoxidation, polymerization of olefins, olefin oxidation (Wacker process) and carbonylation of methanol.

#### **Text Book(s):**

1. W. Kaim and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, (An Introduction and Guide)*, John Wiley and Sons, 1994. (Unit-1)
2. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, Panima Publishing Corporation, 1997. (Unit-2)
3. W. Kaim and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, (An Introduction and Guide)*, John Wiley and Sons, 1994. (Unit-3)
4. G.L. Eichorn, *Inorganic Biochemistry, Volumes 1 & 2*, 2<sup>nd</sup> Ed., Elsevier, 1973. (Unit-4)
5. J.P. Collman, L.S. Hegedus, J.R. Norton, R.G. Finke, *Principles and Applications of Organotransition Metal Chemistry*, University Science Books, 1980. (Unit-5)

#### **Reference Book(s):**

1. J. E. Huheey, *Inorganic Chemistry*, 3<sup>rd</sup> Ed., Harper & Row Publishers, 1983.
2. K.F. Purcell, J.C. Kotz, *Inorganic Chemistry*, Saunders Golden Sunburst Series, 1977.
3. F.A Cotton, G. Wilkinson, *Advanced Inorganic Chemistry*, 5<sup>th</sup> Ed., John Wiley & Sons, 1992.
4. L. Finar, *Organic Chemistry Vol 2, Stereochemistry and the Chemistry of Natural Product*, Dorling Kindersley India (P) Ltd, 2009.

### Question Pattern

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
<b>II</b>	20PCH1CC4	Bio-inorganic and organometallics	6	5						
<b>Course Outcomes (COs)</b>	<b>Programme Outcomes(POs)</b>					<b>Programme Specific Outcomes(PSOs)</b>				
	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PSO1</b>	<b>PSO2</b>	<b>PSO3</b>	<b>PSO4</b>	<b>PSO5</b>
<b>CO1</b>	✓		✓	✓	✓		✓	✓	✓	✓
<b>CO2</b>	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
<b>CO3</b>	✓		✓		✓	✓	✓	✓	✓	✓
<b>CO4</b>	✓		✓		✓	✓	✓	✓		✓
<b>CO5</b>	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER - II

Course Code: 20PCH2CC5  
Instruction Hours: 6  
Credits: 5

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### CORE COURSE 5– SPECTROSCOPY OF ORGANIC MOLECULES

#### Course Outcomes:

- To enable the students to understand, Rotational and Vibrational Spectroscopy.
- To enable the students to correlate the IR stretching frequencies of organic compounds with their functional groups.
- To enable the students to interpret the  $^1\text{H}$  as well as  $^{13}\text{C}$  NMR spectra of organic compounds with individual nuclei (protons/carbons).
- To enable the students to interpret different types of carbons (CH,  $\text{CH}_2$ ,  $\text{CH}_3$  and quaternary C) using  $^{13}\text{C}$  NMR spectral editing and  $^{13}\text{C}$  NMR DEPT techniques. To enable the students to interpret 2D-NMR techniques such as HSQC, HMBC and NOESY.
- To enable the structural elucidation of organic compounds using Mass Spectral data.

#### Unit I

**Rotational and Vibrational Spectroscopy:** Microwave spectroscopy – rotational spectra of diatomic molecules, rigid and non-rigid rotors – Intensity of spectral lines, – Effects of isotopic substitution – Microwave spectra of polyatomic molecules – Linear and symmetric top molecules, techniques and instrumentation.

Introduction - Instrumentation, Sampling techniques - Woodward–Fieser and Scott rules for conjugated dienes and polymers, ketones, aldehydes,  $\alpha$ ,  $\beta$ -unsaturated acids, esters, nitriles, and amides. Differentiation of geometrical isomers and positional isomers – Disubstituted benzene.

#### Unit II

**Advanced Spectroscopy: Infrared Spectroscopy:** Introduction - Instrumentation, Sampling techniques, factors influencing group frequencies – Both internal and external – quantitative studies. Infrared spectra – diatomic molecules, simple harmonic and anharmonic oscillators, – diatomic vibrating rotator, rotation-vibration spectrum of carbon monoxide, – Interaction of rotation and vibration (breakdown of Born – Oppenheimer approximation) – Influence of the rotation on the spectrum of polyatomic molecules, linear and symmetric top molecules, parallel and perpendicular vibrations, influence of nuclear spin. Characterization of functional group frequency ( $-\text{NH}_2$ ,  $-\text{OH}$ ,  $-\text{CH}$ ,  $-\text{CO}$ ,  $-\text{COOH}$ ,  $-\text{CONH}_2$ ,  $-\text{COOR}$  and  $-\text{CHO}$ )

### Unit III

**Nuclear Magnetic Resonance and Their Applications:**  $^1\text{H}$  NMR Spectroscopy – Instrumentation of NMR spectroscopy - Multiplicity – Coupling constant – First order and second order proton. Shielding and Deshielding–Factors affecting chemical shift and factors affecting coupling constant Spin - spin splitting – Dependence of J on dihedral angle – Vicinal and geminal coupling constants – anisotropic effect–double bond, triple bond, aromatic compounds, carbonyl compounds and annulenes. Karplus equation – long range coupling constants, Influence of stereochemical factors on chemical shift of protons. Simplification of complex spectra – double resonance techniques, shifts reagents. Chemical spin decoupling of rapidly exchangeable protons (OH, SH, COOH, NH,  $\text{NH}_2$ ), an elementary treatment of NOE phenomenon. Two interacting nuclei: AB, AX, AA'BB' and. Three interacting nuclei: AMX, ABX, ABC systems. NMR spectrum of cyclopropane, cyclobutane, acetone, acetylacetone, benzamide, dibromoethane, glycol, cyclohexane, aniline, phenol and anisole.

### Unit IV

**$^{13}\text{C}$  NMR &  $^{31}\text{P}$  NMR and 2-D NMR Techniques:**  $^{13}\text{C}$  NMR–difficulties in recording  $^{13}\text{C}$  NMR: Homo nuclear and heteronuclear coupling. Off Resonance decoupled spectrum identification of various types of carbon (functional groups) using  $^{13}\text{C}$  NMR.  $^{31}\text{P}$  NMR– Chemical shift and heteronuclear coupling. Identification of organo phosphorous compounds such as  $(\text{Me})_3\text{P}$ ,  $(\text{EtO})_3\text{P}=\text{O}$  and  $\text{Ph}_3\text{P}$ . P-P bond in NMR. Basic aspects of 2-D NMR techniques: Correlation spectroscopy (COSY). HOMO COSY (HOMCORR:  $^1\text{H}$ - $^1\text{H}$  connectivity,  $^{13}\text{C}$ - $^{13}\text{C}$  connectivity): HSQC and HETERO COSY (HETCORR): HMBC. 2D NOE Correlation Spectroscopy (NOESY).

### Unit V

**Mass Spectrometry:** Origin, basics and bloc diagram of Mass spectrum-Variou types of Ionization techniques- Stability of Molecular ions, Meta stable ions. Base peaks and Isotope peaks. Fragmentation patterns of organic molecules such as benzenes, phenyl halides, phenols, benzyl alcohols, benzyl halides, aliphatic alcohols, aliphatic as well as aromatic aldehydes, ketones, acids, esters and amides. Fragmentation patterns of aliphatic/aromatic nitro and amine compounds. Fragmentation patterns of heterocyclic compounds (furan, pyrrole and pyridine only). McLafferty rearrangements of organicmolecules.

#### Text Book(s):

1. C. N. Banwell and E. M. Mccash, “Fundamentals of Molecular Spectroscopy”, Tata McGraw-Hill Publishing Company Limited, New Delhi, 2009. (Unit-1)
2. Y.R. Sharma, Elementary Organic Spectroscopy: Principles and Chemical Applications, S.Chand Publications, New Delhi, 2012. (Unit-1 & Unit-2)
3. K. Veera Reddy, “Symmetry and Spectroscopy of Molecules”, New Age International Publishers, 2010.(Unit-3)

- P.S.Kalsi, Spectroscopy of Organic Compounds. (Unit-3)
- W. Kemp, Organic Spectroscopy, 3rd Ed., MacMillon, 1994. (Unit-4)
- Gurdeep R Chatwal and Sham K Anand, Spectroscopy, Himalaya Publishing House (2009). (Unit-5).

**Reference Book(s):**

- R. S. Drago, "Physical Methods in Chemistry", New Delhi, East West Press Ltd., 1971.
- B.P. Straughan and S.Walker Spectroscopy Vol.3, Chapman Hall London, 1976.
- P.K.Ghosh, Introduction to Photoelectron Spectroscopy, John Wiley New York, 1989.
- P.M. Silverstein, F. X. Wester, Spectroscopic Identification of Organic Compounds, 6<sup>th</sup>Ed., Wiley 1998.
- G. M. Barrow, "Introduction to Molecular Spectroscopy", Tata-McGraw- Hill Edition, 1993.
- Clegg.W., Crystal structure determination, Oxford University press , New York,1998.
- Stout,G.H., Jensen , L.H. X-ray structure determination : A practical guide , John wiley & sons Publication: New York,1989
- Webpages :**
  - Cambridge Structural Database (CSD) - <http://www.ccdc.cam.ac.uk/products/csd/>
  - Protein Data Bank (PDB) - <http://www.rcsb.org/pdb/home/home.do>

**Question Pattern**

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course					Hours	Credits			
II	20PCH2CC5	Spectroscopy of organic molecules					6	5			
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)					
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	
CO1	✓		✓	✓	✓		✓	✓	✓	✓	
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
CO3	✓		✓		✓	✓	✓	✓	✓	✓	
CO4	✓		✓		✓	✓	✓	✓		✓	
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓	
Number of Matches(✓) = 42 Relationship: High											

Mapping	1-29%	30-59%	60-69%	70-89%	90-100%
Matches	1-14	15-29	30-34	35-44	45-50
Relationship	Very Poor	Poor	Moderate	High	Very High



## SEMESTER - II

Course Code: 20PCH2EC1:1  
Instruction Hours: 6  
Credits: 4

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### ELECTIVE COURSE 1:1– CONCEPTS AND MODELS IN CHEMISTRY

#### Course Outcomes:

- To learn about polymeric bio-organic molecules such as carbohydrates, proteins and nucleic acids.
- To enable the students to understand the importance of trace elements in biological system
- To enable the students to understand the structure and importance of biomolecules such as proteins, nucleic acids and carbohydrate.
- To identify the bonding types.
- Learn the chemical bonding and chemical thermodynamics. Learn chemical kinetics.

#### Unit I

**Bio-Organic Chemistry:** Amino acids and proteins: Structure, classification, nomenclature and function of amino acids, functional groups, isoelectric point – Peptide structure, structural levels of proteins – primary, secondary, tertiary and quaternary, alpha, beta helix – collagen, fibrous and globular proteins.

Nucleic acids: Structures of RNA and DNA.

Enzymes: Co-enzymes – Classification – Characteristics, functions, factors affecting enzyme activity: pH, temperature, substrate concentration. Examples for coenzymes and its functions.

#### Unit II

**Metal Ions in Biology & Chemotherapy:** Metal Ions in Biology - Occurrence and availability of Inorganic elements in Organism - Biological function of inorganic elements - Biological ligands for metal ions – Coordination of Proteins and enzymatic catalysis – Porphyrins and other Macrocycles – Nucleobases, nucleotides and other Nucleic acids as ligands. Metal ion transport and storage – Cobalamines - Metals at the Center of Photosynthesis. Dioxygen transport: Oxygen Transport and Storage through Hemoglobin and Myoglobin. Alternative oxygen Transport in some Lower Animals: Hemerythrin and Hemocyanin.

**Chemotherapy,** Platinum complexes in Cancer therapy – Cisplatin and its mode of action – Cytotoxic compounds of other metals – Gold containing drugs as anti-rheumatic agents and their mode of action. Lithium ion Psychopharmacological drugs.

#### Unit III

**Chemical Bonding:** Atomic structure – Core and valence electrons – periodicity – valence shells and chemical reactivity – valence and chemical formulas – covalent, ionic and co-

ordinate bonds – hydrogen bonds – non-covalent interactions – electronic and molecular structure -  $\sigma$ ,  $\pi$  and  $\delta$  bonds – bond parameters – conformation, configuration – various representations – macromolecules and three dimensional structures.

#### **Unit IV**

**Chemical Thermodynamics:** Energy and the First Law of Thermodynamics, Conservation of energy-principle, work and heat, enthalpy, exothermic and endothermic reactions,  $C_p$  &  $C_v$ , Hess's law of heat summation, use of standard enthalpies of formation – Entropy and the second law of Thermodynamics, Kelvin and Clausius statements of Second Law, definition of entropy, spontaneity and reversibility, entropy change of the system, molecular basis of entropy, free energy and chemical equilibrium, Factors affecting equilibrium.

#### **Unit V**

**Chemical Kinetics:** Rate of Reaction, order of reaction - derivation of rate equation for first order reaction, Determination of rate equation by isolation method – Effect of temperature on reaction rate - Arrhenius equation - Enzyme Kinetics – Michaelis - Menten equation - Salt effect on reaction rate (derivation not needed).

#### **Text Book(s):**

1. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Purnima Publishing Company, 1997.(Unit-1)
2. Geoffrey L. Zubay, William W. Parson and Dennis E. Vance, Principles of Biochemistry- McGraw-Hill Education,1995. (Unit-2)
3. D. E. Douglas, D.H. McDaniel and J. J. Alexander, Concepts and Models in Inorganic Chemistry, 3<sup>rd</sup> Ed, 1994. (Unit-3)
4. S. Glasstone, Thermodynamics for Chemists, Affiliated East West Press, New Delhi,1960. (Unit-4)
5. Gordon M. Barrow, Physical Chemistry, Tata McGraw Hill, 1994.(Unit-5)

#### **Reference Book(s):**

1. B.H. Mahan, University chemistry, Narosa Publishers.
2. Bruce H. Mahan, University chemistry, Narosa Publishers.
3. David L. Nelson and Michael M. Cox, Lehninger Principles of Biochemistry, W H Freeman, 2017.
4. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6<sup>th</sup> Ed., Pearson, 1992.
5. I.L. Finar, Organic Chemistry, Vol.II, 5<sup>th</sup> ed., ELBS 1975.
6. J.E. Huheey, Inorganic Chemistry, 3<sup>rd</sup> Ed., Harper & Row publisher, 1983.
7. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley
8. C.H. Snyder, The extra-ordinary chemistry of ordinary things, John Wiley, 1992.
9. P.W. Atkins, Physical Chemistry, ELBS and Oxford University Press, 1998.

### Question Pattern

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
<b>II</b>	20PCH2EC1:1	Concepts and models in chemistry	6	4						
<b>Course Outcomes (COs)</b>	<b>Programme Outcomes(POs)</b>					<b>Programme Specific Outcomes(PSOs)</b>				
	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PSO1</b>	<b>PSO2</b>	<b>PSO3</b>	<b>PSO4</b>	<b>PSO5</b>
<b>CO1</b>	✓		✓	✓	✓		✓	✓	✓	✓
<b>CO2</b>	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
<b>CO3</b>	✓		✓		✓	✓	✓	✓	✓	✓
<b>CO4</b>	✓		✓		✓	✓	✓	✓		✓
<b>CO5</b>	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42    Relationship: High										

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER - II

Course Code: 20PCH2EC1:2  
Instruction Hours: 6  
Credits: 4

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### ELECTIVE COURSE 1:2– METALLO PROTEINS, ENZYMES AND NATURAL PRODUCTS

#### Course Outcomes:

- To enable the students to understand the structure and importance of biomolecules such as of amino acids and proteins.
- To enable the students to understand the structure and functions of various types of metalloenzymes.
- To enable the students to understand the structure and importance of biomolecules such as, nucleic acids and proteins synthesis.
- To enable the students to understand the structure and importance of antibiotics and vitamins.
- To enable the students to understand the structural elucidation and biosynthesis of alkaloids and terpenes.

#### Unit I

**Amino Acids and Proteins:** Structure, classification, synthesis and properties of amino acids, isoelectric point, biosynthesis of amino acids. Peptides: oligo- and polypeptides, geometry of peptide linkage, N-terminal and C-terminal residue analysis, synthesis of peptides-amino and carboxyl protecting groups-solid phase peptide synthesis. Proteins: classification and properties (denaturation, isoelectric point and electrophoresis), primary, secondary, tertiary and quaternary structures of proteins, collagen and triple helix.

#### Unit II

**Enzymes and Cofactors:** Mechanism of enzyme catalysis, Factors influencing enzyme action, Examples of typical enzyme mechanisms: chymotrypsin, ribonuclease and lysozyme, Enzyme-catalyzed addition, elimination, condensation, carboxylation and decarboxylation, isomerisation, group transfer and rearrangement reactions-structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate,  $\text{NAD}^+$ ,  $\text{NADP}^+$ , FMN, FAD, lipoic acid and Vitamin  $\text{B}_{12}$ . Mechanisms of reactions catalysed by the above cofactors.

#### Unit III

**Nucleic Acids and Protein Synthesis :** Nucleotides and nucleosides, DNA: primary and secondary structure-replication of DNA. RNA and protein synthesis: Messenger RNA synthesis-transcription, Ribosomes-rRNA, Transfer RNA, genetic code-translation. Determination of base sequence of DNA. Polymerase Chain Reaction (PCR). Antisense technology in chemotherapy and other nucleic acid-targeted drugs-intercalators, sequence specific drugs. A brief account of ribosome and iRNA.

#### Unit IV

**Antibiotics and Vitamins:** Biomolecules: Antibiotics and vitamins: A detailed study of structure, stereochemistry and synthesis of penicillin, cephalosporin. Chemistry and physiological action of ascorbic acid, thiamin, riboflavin and pyridoxine – Elementary aspect of vitamin A, E, K and B<sub>12</sub>.

#### Unit V

**Natural Products: Alkaloids:** Synthesis and reactions of the following: Tropine, Cinchonine, Morphine, Papaverine and structural elucidation of Reserpine ( synthesis not expected).

**Terpenes:** Structural elucidation, medicinal values and synthesis of alpha – pinene, camphor and zingiberene.

#### Text Book(s):

1. Bioorganic Chemistry: A Chemical approach to Enzyme action, Hermann Dugas and C.Penny, Springer-Verlag. (Unit-1)
2. David L. Nelson and Michael M. Cox, Leninger Principles of Biochemistry, W H Freeman, 2017. (Unit-2 & Unit-3 )
3. Geoffrey L. Zubay, William W. Parson and Dennis E. Vance, Principles of Biochemistry- McGraw-Hill Education, 1995. (Unit-4)
4. I. L. Finar, Organic Chemistry Vol. I & II, 6<sup>th</sup> edition, Pearson Education, Dorling Kindersley India (P) Ltd, 2009. (Unit - 5).

#### Reference Book(s):

1. Fundamentals of Enzymology, N.C. Price and L. Stevens, Oxford University Press.
2. Designing Organic Synthesis: The Disconnection Approach by Stuart Warren, Wiley, 2nd edition, 1984.
3. Asymmetric Synthesis by H. B. Kagan, Thieme Medical Publishers, 2003.
4. Advanced Organic Chemistry: Part-A and Part-B by Francis A. Carey and Richard B. Sundberg, Springer, 5th edition, 2007.
5. Koji Nakanishi, Toshio Goto and Shô, Itô, Natural Product Chemistry, Vol. I, Academic Press, 1974.
6. A. Newman, Chemistry of Terpenes and Terpenoids, Academic Press, 1972.

#### Question Pattern

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
II	20PCH2EC1:2	Metallo proteins, enzymes and natural products	6	4						
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓		✓	✓	✓		✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO3	✓		✓		✓	✓	✓	✓	✓	✓
CO4	✓		✓		✓	✓	✓	✓		✓
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

Mapping	1-29%	30-59%	60-69%	70-89%	90-100%
Matches	1-14	15-29	30-34	35-44	45-50
Relationship	Very Poor	Poor	Moderate	High	Very High

## SEMESTER - II

Course Code: 20PCH2EC1:3  
Instruction Hours: 6  
Credits: 4

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### ELECTIVE COURSE 1:3– SUPRAMOLECULAR CHEMISTRY

#### Course Outcomes:

- To enable the students to understand fundamentals of supramolecules.
- Understand concepts Metallo Organic Frameworks
- To enable the students to understand co-receptor molecules and multiple recognition
- To enable the students to understand the concept of supramolecular reactivity and catalysis.
- To learn the designs various types of supramolecular devices

#### Unit I

**Concepts of Supramolecular Chemistry:** Concepts and languages of supramolecular chemistry – various types of noncovalent interactions – hydrogen bonds, C-H...X interactions, halogen bonds – $\pi$ - $\pi$  interactions, non-bonded interactions – various types of molecular recognition.

Crystal engineering of organic solids – hydrogen bonded supramolecular patterns involving water / carboxyl / halide motifs – concepts of different types of synthons based on non-covalent interactions – principles of crystal engineering and non-covalent synthesis – polymorphism and pseudopolymorphism – supramolecular isomorphism / polymorphism – crystal engineering of pharmaceutical phases.

#### Unit II

**Metallo Organic Frameworks:** M.O.F (Metallo Organic Frameworks) – organometallic systems – combinations of different interactions to design molecular rods, triangles, ladders, networks, etc. – design of nanoporous solids – interligand hydrogen bonds in metal complexes – implications for drug design – crystal engineering of NLO materials, OLED.

#### Unit III

**Co-receptor Molecules and Multiple Recognition:** Dinuclear and polynuclear metal ion cryptates – linear recognition of molecular length by ditopic co-receptors – heterotopic co-receptors – cyclophane receptors, amphiphilic receptors and large molecular cages – multiple recognition in metallo-receptors – supramolecular dynamics.

#### Unit IV

**Supramolecular Reactivity and Catalysis:** Catalysis by reactive macrocyclic cation receptor molecules – catalysis by reactive anion receptor molecules – catalysis with cyclophane type receptors – supramolecular metallocatalysis – cocatalysis – catalysis of

synthetic reactions– biomolecular and abiotic catalysis. Supramolecular chemistry in solution – cyclodextrin, micelles, dendrimers, gelators – classification and typical reactions – applications.

## **Unit V**

**Supramolecular Devices:** Supramolecular devices and sensors – various types of supramolecular devices– an overview – supramolecular photochemistry – molecular and supramolecular photonic devices – light conversion and energy transfer devices– molecular and supramolecular electronic devices – electronic conducting devices – molecular wires, modified and switchable molecular wires – molecular and supramolecular ionic devices – tubular mesophases, molecular protonics – switching devices – electro-photo switch – ion and molecule sensors– role of supramolecular chemistry in the development of nanoscience and technology.

### **Text Book(s):**

1. Jonathan W. Steed, David R. Turner and Karl J. Wallace, Core Concepts in Supramolecular Chemistry and Nanochemistry, John Wiley & Sons, Ltd, (2007). (Unit-1)
2. J. M. Lehn, Supramolecular Chemistry; VCH, Weinheim, Germany, 1995. (Unit-2)
3. G. R. Desiraju, Crystal Engineering: The Design of Organic Solids; Elsevier, United States, 1989. (Unit-3).
4. G. A Jeffrey, Introduction to Hydrogen Bonding; Oxford University Press: UK, 1997. (Unit-3).
5. J. W. Steed and J. L. Atwood, Supramolecular Chemistry, 2nd edition John Wiley & Sons (2009). (Unit-4 )
6. J. M. Lehn, Transition Metals in Supramolecular Chemistry; John Wiley and Sons: New York, 1999. (Unit-5)

### **Reference Book(s):**

1. J. M. Lehn, Supramolecular Chemistry; VCH, Weinheim, Germany, 1995.
2. G. R. Desiraju, Crystal Engineering: The Design of Organic Solids; Elsevier, United States, 1989.
3. G. R. Desiraju, and T. Steiner, The Weak Hydrogen Bond in Structural Chemistry and Biology; Oxford University Press, Oxford, 1999.
4. J. M. Lehn, Transition Metals in Supramolecular Chemistry; John Wiley and Sons: New York, 1999.
5. G. R. Desiraju, Current Science; 2001, 81, 1038.
6. Web source:
  - (i) Crystal Growth and Design,  
<http://www.pubs.acs.org/journals/cgdefu/index.html>
  - (ii) Crystal Engineering  
Communication <http://www.rsc.org/Publishing/Journals/ce/index.asp>



### Question Pattern

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
<b>II</b>	20PCH2EC1:3	Supramolecular chemistry	6	4						
<b>Course Outcomes (COs)</b>	<b>Programme Outcomes(POs)</b>					<b>Programme Specific Outcomes(PSOs)</b>				
	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PSO1</b>	<b>PSO2</b>	<b>PSO3</b>	<b>PSO4</b>	<b>PSO5</b>
<b>CO1</b>	✓		✓	✓	✓		✓	✓	✓	✓
<b>CO2</b>	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
<b>CO3</b>	✓		✓		✓	✓	✓	✓	✓	✓
<b>CO4</b>	✓		✓		✓	✓	✓	✓		✓
<b>CO5</b>	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42    Relationship: High										

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER - II

Course Code: 20PCH2CP3

Instruction Hours: 6

Credits: 4

Exam Hours: 6

Internal Marks: 40

External Marks:60

### CORE COURSE PRACTICAL 3 – ORGANIC ESTIMATION AND DOUBLE STAGE PREPARATIONS – PRACTICAL

#### Course Outcomes:

- To enable the students to learn about estimation of organic compounds. Be able to learn quantitative analysis of organic compounds.
- Synthesize the students to understand simple double stage preparations preparation of organic compounds.
- Synthesize the students to understand isolation of organic compounds.
- To enable the students to learn about find out melting point of organic compounds.
- To enable the students to learn about purification of organic compounds.

#### 1. Estimations

1. Estimation of Aniline
2. Estimation of Phenol
3. Estimation of Methyl ketones
4. Estimation of Glucose
5. Estimation of Hydroxyl group
6. Estimation of Nitro group
7. Saponification Reaction Value

#### 2. Preparation and Isolation

1. Aniline to tribromoaniline to tribromobenzene
2. Methyl benzoate to methyl-*m*-nitrobenzoate to methyl-*m*-nitrobenzoic acid
3. Methyl salicylate to salicylic acid to acetyl salicylic acid
4. Chlorobenzene to dinitrochlorobenzene to 2,4-dinitrophenylhydrazine
5. Hydroquinone to *p*-benzoquinone to 5-hydroxy-1,3-benzoxathiaole to 5-acetoxy-1,3-benzoxathiaole-2-one
6. Extraction of Eugenol from clove

#### Reference Book(s):

1. J. Mohan, Organic Analytical Chemistry, Theory and Practice, Narosa, 2003.
2. V.K. Ahluwalia, P. Bhagat, R. Aggarwal, Laboratory Techniques in Organic Chemistry, I.K. International, 2005.
3. N.S. Gnanaprakasam, G. Ramamurthy, Organic Chemistry Lab Manual, S.V. Printers, 1987.
4. A.I. Vogel, A.R. Tatchell, B.S. Furnis, A.J. Hannaford, P.W.G. Smith, Vogel's Textbook of Practical Organic Chemistry, 5<sup>th</sup> Ed., Prentice Hall, 19

### Scheme of Valuation

Criteria		Marks	
Record		5	
Aim and tabulation		10	
Organic double stage preparation [25]		Organic estimation 20]	
Stage I	10	Error	Marks
		< 1 %	20
Stage II	15	1-2%	15
		2-3%	10
		3%	5

#### Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course					Hours	Credits			
II	20PCH2CP3	Organic estimation and double stage preparations – practical					6	4			
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)					
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	
CO1	✓		✓	✓	✓		✓	✓	✓	✓	
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
CO3	✓		✓		✓	✓	✓	✓	✓	✓	
CO4	✓		✓		✓	✓	✓	✓		✓	
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓	
Number of Matches(✓) = 42 Relationship: High											

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER - II

Course Code: 20PCH2CP4

Instruction Hours: 6

Credits: 4

Exam Hours: 6

Internal Marks: 40

External Marks:60

### **CORE COURSE PRACTICAL 4 – INORGANIC ESTIMATION AND COMPLEX PREPARATIONS – PRACTICAL**

#### **Course Outcomes:**

- To enable the students to learn about gravimetric estimation.
- Synthesize the students to understand preparations of coordination complex.
- Synthesize the students to understand characterization of coordination complex.
- To enable the students to learn about quantitative analysis of cations.
- To enable the students to learn about purification of coordination compounds.

#### **1. Volumetric and gravimetric analysis of a solution containing two cations**

1. Copper and Nickel
2. Copper and Zinc
3. Ferrous and Ferric ions
4. Barium and Calcium

#### **2. Preparations and Characterization of Co-ordination Complexes**

1. Tris(thiourea)copper(I) sulphate
2. Tetramminecopper(II) sulphate
3. Pentathioureadicuprous nitrate
4. Potassium trioxalato ferrate
5. Potassium trioxalatoaluminate
6. Potassium trioxalatochromate
7. Cis-Potassium dioxalato diaquochromate
8. Hexathiourea plumbum nitrate
9. Hexamminecobalt(III) chloride

#### **Reference Book(s):**

1. A.I. Vogel's, Quantitative Inorganic Analysis, 5<sup>th</sup> Ed., Prentice Hall, 1996.

**Scheme of valuation**

Criteria		Marks	
<b>Record</b>		<b>5</b>	
<b>Aim and tabulation</b>		<b>10</b>	
<b>Inorganic preparation [15]</b>		<b>Gravimetry 30</b>	
<b>Bulk precipitate</b>	15	<b>Error</b>	<b>Marks</b>
		< 1 %	<b>30</b>
		1-2%	25
		2-3%	15
		3%	10

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course					Hours	Credits		
<b>II</b>	20PCH2CP4	Inorganic estimation and complex preparations – practical					6	4		
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
<b>CO1</b>	✓		✓	✓	✓		✓	✓	✓	✓
<b>CO2</b>	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
<b>CO3</b>	✓		✓		✓	✓	✓	✓	✓	✓
<b>CO4</b>	✓		✓		✓	✓	✓	✓		✓
<b>CO5</b>	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER – III

Course Code: 20PCH3CC6  
Instruction Hours: 6  
Credits: 5

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### CORE COURSE 6 - PHOTOCHEMISTRY, PERICYCLIC REACTIONS, HETEROCYCLES AND REAGENTS

#### Course Outcomes:

- Learn the knowledge in organic photochemistry
- Learn the reagents and reaction of organic compounds
- Learn the theoretical aspect of organic synthesis
- The students will be able to introduce about basic chemistry of the heterocyclic.
- The students will get familiar with particular properties and reactions for the most important heterocyclic as well as different systems of nomenclature.

#### UNIT – I: Organic Photochemistry (18 – Hours)

Fundamental concepts – Jablonski diagram – energy transfer characteristics of photo sensitization – characteristics of photo reactions of ketones - Norrish type I and II – reactions – photochemistry of alkenes, dienes and aromatic compounds – reactions of unactivated centres – photo additions – Paterno- Buchi reaction. Photo substitution - Barton reaction – Hoffmann – Löffler - Freytag reaction. Photo rearrangement - Photo – Fries and di -  $\pi$  methane rearrangements.

#### UNIT II: Orbital Symmetry & Pericyclic Reactions (18 – Hours)

Pericyclic reactions – Concerted reactions – Symmetry properties of molecular orbital - Electrocyclic reactions- correlation diagram and Frontier molecular orbital (FMO) approach – Woodward Hoffmann rules. Cycloaddition reactions-Diels Alder reaction- stereochemical modes: suprafacial and antarafacial processes- orbital symmetry in cycloaddition reaction: correlation diagrams and FMO method. Sigmatropic rearrangements – analysis – Cope and Claisen rearrangements Applications of FMO methods to pericyclic reactions.

#### UNIT-III: Heterocycles and their Reactivity (18 – Hours)

Structure, synthesis and their reaction of the following systems; a) One heteroatom - Pyrrole, Furan, Thiophene, Pyridine; b) Benzo fused Heterocycles - Indole, Quinoline; Two heteroatom - Pyrazole, Imidazole, Pyrimidine, Pyrazine.

#### UNIT-IV: Named Reactions and Strategic Applications (18–Hours)

Bamford-Stevens Reaction – Baylis-Hillman Reaction – Biginelli Reaction — Henry Reaction – Hosomi-Sakurai Reaction – Hunsdiecker Reaction –Mukaiyama Aldol

Addition – Nazarov Cyclization – Peterson Olefination – Prevost Reaction – Prins Reaction – Ugi reaction - Wittig reaction and its modifications. Palladium based reactions: Fukuyama Coupling – Heck Reaction – Hiyama Coupling – Stille Coupling – Suzuki Coupling – Tsuji-Trost Reaction.

#### **UNIT V: Reagents in Organic Synthesis**

**(18 – Hours)**

Catalytic hydrogenation and dehydrogenation – Reduction with LAH, NaBH<sub>4</sub>, tritertiarybutoxy aluminum hydride, NaCNBH<sub>3</sub>, tributyltin hydride, Me<sub>3</sub>SiCN, alkali metals for reduction, reductions with hydrazines. Osmium tetroxide – Sharpless asymmetric epoxidation – Chromyl chloride – Ozone – DDQ – Dioxiranes – Lead tetraacetate – Selenium dioxide – Gilman reagents - Dithione – DMSO either with Ac<sub>2</sub>O or oxalyl chloride – Dess-Martin reagent – LDA – Phase transfer catalysis (PTC) – Merrifield resin – Baker’s yeast.

#### **Text Books:**

1. R.K. Bansal, Heterocyclic chemistry- Syntheses, Reactions and Mechanisms, Wiley Eastern Ltd, 1990.
2. S.M.Mukherji and S.P.Singh, Reaction Mechanism in Organic Chemistry, 3<sup>rd</sup> edition, Macmillan, 2010.
3. Ahluwalia, V K, Textbook of Organic Chemistry, New Delhi: Narosa Publishing, 2000.

#### **References:**

1. H.O. House, Modern Synthetic Reactions, 2<sup>nd</sup> Ed., W. A. Benjamin, 1972.
2. F.A. Carey, R.J. Sundberg, Advanced Organic Chemistry, Parts A & B, 5<sup>th</sup> Ed., Springer, 2007.
3. T. L. Gilchrist, Heterocyclic Chemistry, 3<sup>rd</sup> Ed., Prentice Hall, 1997.
4. K. Mackie, M. Smith, Guide Book to Organic Synthesis, ELBS, England 1982.
5. L. Kurti, B. Czako, Strategic Applications of Named Reactions in Organic Synthesis, Elsevier, 2005.
6. Hassner, C. Stumer, Organic Synthesis Based on Name and Unnamed Reactions, Elsevier Science Ltd., UK, 1994.
7. R.O.C. Norman – “Principles of Organic Synthesis” – 2nd Ed., (1986), Chapman and Hall Publications, New York.
8. Also refer: <http://www.organic-chemistry.org/>; <http://www.organicworldwide.net>.

#### **Question Pattern**

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
III	20PCH3CC6	Photochemistry, pericyclic reactions, heterocycles and reagents	6	5						
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓		✓	✓	✓		✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO3	✓		✓		✓	✓	✓	✓	✓	✓
CO4	✓		✓		✓	✓	✓	✓		✓
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High



## SEMESTER – III

Course Code: 20PCH3CC7  
Instruction Hours: 6  
Credits: 5

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### CORE COURSE 7 - SPECTROSCOPY OF COORDINATION COMPLEXES

#### Course Outcomes:

- Identify molecular geometries associated with various d-orbital splitting patterns. Learn electronic spectroscopy of metal complexes.
- Predict electron configurations of split d orbitals for selected transition metal atoms or ions
- Learn detail IR, Raman and NMR of inorganic compounds
- Learn the EPR, Mossbauer and magnetic properties of metal complexes.
- Determine the nature of proton and determine number of equivalent proton in a molecule from proton NMR spectra.

#### UNIT- I: Electronic Spectroscopy

(18 – Hours)

Electronic configuration-quantum numbers spin-spin coupling, orbit-orbit coupling and spin-orbit coupling, microstates, terms, Mulliken symbols for microstates and energy level splitting for  $d^1 - d^9$  ions in cubic and square fields – selection rule for electronic spectra – Orgel diagram and Tanabe-Sugano diagram, evaluation of  $10Dq$  and  $\beta$  for octahedral complexes of cobalt, nickel and  $[\text{Ru}(\text{bipy})_3]^{2+}$ -intensity of bands – effect of distortion and spin-orbit coupling on spectra – applications to simple coordination compounds – charge transfer spectra – L-M and M-L charge transfer transition. ORD, CD and MCD – principle and applications to metal complexes.

#### UNIT II: Infrared and Raman Spectroscopy

(18 – Hours)

Conditions for IR active, vibrations in simple molecules ( $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ) and their symmetry notation for molecular vibrations – group vibrations and the limitations – combined uses of IR and Raman spectroscopy in the structural elucidation of simple molecules like  $\text{N}_2\text{O}$ ,  $\text{ClF}_3$ ,  $\text{NO}_3$  – effect of coordination on ligand vibrations – uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate and dimethyl sulfoxide. Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal carbonyls with reference to the nature of bonding – geometry and number of C-O stretching vibrations (group theoretical treatment) – applications of Raman spectroscopy.

**UNIT III: NMR Spectroscopy (18 – Hours)**

NMR spectroscopy – theory of NMR spectra, number of NMR signals – chemical shifts, factors affecting the chemical shift values and coupling constants involving different nuclei ( $^1\text{H}$ ,  $^{31}\text{P}$ ,  $^{13}\text{C}$ )– Effect of quadrupolar nuclei ( $^2\text{H}$ ,  $^{10}\text{B}$ ,  $^{11}\text{B}$ ) on the  $^1\text{H}$  NMR spectra.  $^{13}\text{C}$  NMR – proton decoupled and off – resonance  $^{13}\text{C}$  NMR spectra – factors affecting the  $^{13}\text{C}$  NMR chemical shifts - Systems with chemical exchange – study of fluxional behaviour of molecules – NMR of paramagnetic molecules.

**UNIT IV: EPR Spectroscopy and Magnetic properties (18 – Hours)**

Theory of EPR spectroscopy – spin densities and McConnell relationship – factors affecting the magnitude of g and A tensors in metal species – zero-field splitting and Kramers degeneracy – spectra of V(II), Mn(II), and Cu(II) complexes – applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions. Magnetic properties – types of magnetism – dia-, para-, ferro- and antiferromagnetism – magnetic properties of free ions – first-order Zeeman effect – second-order Zeeman effect – states  $kT \ll \text{states} \ll kT$  – determination of magnetic moments and their applications to the elucidation of structures of inorganic compounds.

**UNIT V: Mossbauer and NQR Spectroscopy (18 – Hours)**

Introduction, principle, instrumentation, recoil energy, Doppler effect, number of MB signals, isomer shift, quadrupole splitting, magnetic hyperfine splitting- applications to  $^{57}\text{Fe}$ , and  $^{119}\text{Sn}$  compounds. NQR spectroscopy – characteristics of quadrupolar nucleus – effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – applications of NQR spectroscopy.

**Text Books:**

1. C. N. Banwell and E. M. Mccash, “Fundamentals of Molecular Spectroscopy”, Tata McGraw-Hill Publishing Company Limited, New Delhi, 2009.
2. Y. R. Sharma, Elementary Organic Spectroscopy – Principles and Chemical Applications; S. Chand and Co., New Delhi, 1992.
3. P. S. Kalsi, Spectroscopy of Organic Compounds; 6th Ed., New Age International Publishers, New Delhi, 2004.

**References:**

1. R. S. Drago, Physical Methods in Inorganic Chemistry; Affiliated East-West Press Pvt. Ltd., New Delhi, 2012.
2. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Ed., Wiley-Eastern Company, New Delhi, 1999.
3. P. J. Wheatley, The Determination of Molecular Structure; 2nd Ed., Dover Publications, Mineola, 1981.
4. G. J. Leigh, N. Winterton, Modern Coordination Chemistry; Royal Society of Chemistry, UK, 2002.
5. E. A. V. Ebsworth, Structural Methods in Inorganic Chemistry; 3rd Ed., ELBS, Great Britain, 1987.

6. W. Kemp, Organic Spectroscopy; 3rd Ed., Palgrave, New York, 2011.
7. J. R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds, PHI Learning, New Delhi, 2009.

### Question Pattern

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
<b>III</b>	20PCH3CC7	Spectroscopy of coordination complexes	6	5						
<b>Course Outcomes (COs)</b>	<b>Programme Outcomes(POs)</b>					<b>Programme Specific Outcomes(PSOs)</b>				
	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PSO1</b>	<b>PSO2</b>	<b>PSO3</b>	<b>PSO4</b>	<b>PSO5</b>
<b>CO1</b>	✓		✓	✓	✓		✓	✓	✓	✓
<b>CO2</b>	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
<b>CO3</b>	✓		✓		✓	✓	✓	✓	✓	✓
<b>CO4</b>	✓		✓		✓	✓	✓	✓		✓
<b>CO5</b>	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER – III

Course Code: 20PCH3EC2:1

Instruction Hours: 6

Credits: 4

Exam Hours: 3

Internal Marks: 25

External Marks: 75

### **ELECTIVE COURSE 2:1 - CRYSTAL STRUCTURE, ORGANIC SOLID STATE AND OPTICAL PROPERTIES**

#### **Course Outcomes:**

- An overview of the synthesis and applications of inorganic materials
- Learn to crystal structures of few inorganic solids.
- Learn the applications of magnetic materials.
- Structure and compound identification in the solid state
- Learn the chemistry of organic solids.

#### **UNIT - I: Crystal Structure and Crystal Engineering of Organic Solids (18 – Hours)**

Types of close packing – hcp and ccp – packing efficiency – SC, BCC, and FCC, radius ratio rule – applications – polyhedral description of solids – structure types: Na<sub>2</sub>O, Cs<sub>2</sub>O, rutile, perovskite (ABO<sub>3</sub>), ReO<sub>3</sub>, K<sub>2</sub>NiF<sub>4</sub>, spinels and antispinel. Supramolecular chemistry- motifs – concepts of different types of synthons based on non-covalent interactions – principles of crystal engineering and non-covalent synthesis – polymorphism and pseudopolymorphism – supramolecular isomorphism, polymorphism and crystal engineering of pharmaceutical phases.

#### **UNIT- II: Preparative Methods in Solid State Chemistry (18 – Hours)**

Experimental procedure, coprecipitation as a precursor to solid state reaction, other precursor methods, kinetics of solid state reactions – crystallizations of solutions, melts, glasses and gels, solutions and gels: zeolite synthesis – precipitation from solution or melt: flux method, epitaxial growth of thin layers, verneuil flame fusion method. Graphite intercalation compounds, transition metal dichalcogenide and other intercalation compounds, ion exchange reaction, synthesis of new metastable phases by ‘Chimie Douce’. Electrochemical reduction methods – preparation of thin films, chemical and electrochemical methods, physical methods – growth of single crystals, Czochralski method, Bridgman-Stockbarger methods – zone melting.

#### **UNIT- III: Chemistry Of Solid State: Diffraction Methods (18 – Hours)**

X-Ray diffraction by single crystal method – space groups – systematic absences in X-ray data and identification of lattice types, glide planes and screw axes – X-ray intensities – structure factor and its relation to intensity and electron density – phase problem – structure solution by heavy atom method and direct method – determination of absolute configuration of molecules – a brief account of Cambridge Structural Database (CSD) and Protein Data Bank (PDB).

**UNIT- IV: Magnetic Materials and Optical Properties (18 – Hours)**

Selected examples of magnetic materials and their properties – metals and alloys, transition metal oxides, spinels, garnets, ilmenite and perovskites. Magnetoplumbites – applications – structure/property relations – transformer, information storage, magnetic bubble memory devices, permanent magnets. Luminescence, Lasers and phosphors – definitions and general comments, configurational coordinate model, some phosphor materials, anti-Stokes phosphors – lasers – the ruby laser, Neodymium lasers

**UNIT- V: Organic Solid State Chemistry (18 – Hours)**

Topochemical control of solid state organic reactions – intramolecular reactions – conformational effects – intermolecular reactions – molecular packing effects – photodimerization of 2-ethoxycinnamic acid ( $\alpha$  form,  $\beta$  form,  $\gamma$  form) – photopolymerization of 2,5-distyrylpyrazine – photopolymerizations of diacetylenes. Asymmetric syntheses – dimerization of anthracene – control of molecular packing arrangements. Organic reactions within inorganic host structures – electrically conductive organic solids – organic metals, conjugated systems, doped polyacetylene, polyparaphenylene, polypyrrole – organic charge transfer complexes – new superconductors

**Text Books:**

1. James E. Huheey, Ellen A. Keiter and Richard L. Keiter – “Inorganic Chemistry Principles of Structure and Reactivity”, 4 th Edn., Pearson Education, 11th Impression, 2011.
2. R. West, Solid State Chemistry and Its Applications; 2nd Ed., John Wiley and sons, New York, 2014 (Unit III – V).

**References:**

1. J. M. Lehn, Supramolecular Chemistry; VCH, Weinheim, 1995.
2. G. R. Desiraju, Crystal Engineering: The Design of Organic Solids; Elsevier, Amsterdam, 1989.
3. G. R. Desiraju, and T. Steiner, The Weak Hydrogen Bond in Structural Chemistry and Biology; Oxford University Press: Oxford, 2002.
4. G. A. Jeffrey, Introduction to Hydrogen Bonding; Oxford University Press, New York, 1997.
5. J. M. Lehn, Transition Metals in Supramolecular Chemistry; Vol 5, John Wiley and Sons, New York, 1999.

**Question Pattern**

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
III	20PCH3EC2:1	Crystal structure, organic solid state and optical properties	6	4						
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓		✓	✓	✓		✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO3	✓		✓		✓	✓	✓	✓	✓	✓
CO4	✓		✓		✓	✓	✓	✓		✓
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

Mapping	1-29%	30-59%	60-69%	70-89%	90-100%
Matches	1-14	15-29	30-34	35-44	45-50
Relationship	Very Poor	Poor	Moderate	High	Very High

## SEMESTER-III

Course Code: 20PCH3EC2:2  
Instruction Hours: 6  
Credits: 4

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### ELECTIVE COURSE 2:2 - SELECTED TOPICS IN CHEMISTRY – I

#### Course Outcomes:

- Able to interpret <sup>1</sup>H-NMR, IR, MASS and UV spectral properties for a given compound.
- Learn the general information about spectroscopy, amino acids, proteins and ionic concept
- Expertize in writing conformational structures of carbohydrates and in determination of amino acid sequence in proteins.
- Students are able to recognize and balance oxidation-reduction reactions
- Learn the oxidation-reduction reactions, metals in biology

#### UNIT- I: Introduction to Spectroscopy

(18 – Hours)

Electromagnetic radiations and spectroscopy – UV-Visible spectroscopy: Theory – Beer-Lambert's law (derivation not required) – Important terminologies: molar absorptivity, chromophore, auxochrome, bathochromic shift, hypsochromic shift – Instrumentation (block diagram only) – Spectra of acetone and benzene – IR spectroscopy: Theory – Molecular vibrations – Characteristic group frequencies – Instrumentation (block diagram only) – Spectra of acetone and ethanol – NMR spectroscopy: Theory – Chemical shift – Spin-spin splitting – Instrumentation (block diagram only) – Spectra of ethanol and ethyl benzene – Mass spectroscopy: Introduction – Application for determination mass for simple organic molecules.

#### UNIT - II: Amino acids and Proteins

(18 – Hours)

Structure – Classification – Nomenclature – Functional groups – Isoelectric point – Peptide structure – Structural levels of proteins – Primary, secondary, tertiary and quaternary, alpha, beta helix – Collagen, fibrous and globular proteins – Nucleic acids: Structure of RNA and DNA.

**Enzymes** Classification of enzymes – Basic aspects of enzymes – Factors affecting enzyme activity: pH, temperature, substrate concentration – Examples of Coenzymes and its function.

#### UNIT-III: Ionic equilibria in aqueous solution

(18 – Hours)

Acids and bases, Arrhenius theory, Lowry - Bronsted Concept, Lewis concept – Self ionization of water – Weak acids and bases, dissociation constants – hydrolysis – buffer solutions, action of buffers – acid base indicators – Acid-base titrations – basics, Complex ion equilibria.

**UINT- IV: Oxidation – Reduction reactions and redox potentials (18 – Hours)**

Concept of Oxidation state (Oxidation number), rules to assign oxidation states in polyatomic molecule – Half-reaction concept – balancing oxidation – reductions by half – reaction method – Galvanic cells, various types of electrode – Standard electrode (cell) potential – various conventions regarding half cell potentials – Nernst equation – Chemical and concentration cells – cell potentials and equilibrium constants.

**UINT- V: Metals in biology (18 – Hours)**

Occurrence and availability of inorganic elements in organism – Biological function of inorganic elements – Biological ligands for metal ions – Coordination of proteins and enzymatic catalysis – Porphyrins and other macrocycles – Nucleobases, nucleotides and other nucleic acids as ligands – Metal ion transport and storage – Dioxygen transport – Oxygen transport and storage through hemoglobin and myoglobin – Alternative oxygen transport in some lower animals – Hemerythrin and hemocyanin.

**Text Books:**

1. W. Kemp, Organic Spectroscopy, 3<sup>rd</sup> Ed., MacMillan, 1994.
2. D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3<sup>rd</sup> Ed., Brooks Cole, 2000.
3. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6<sup>th</sup> Ed., Pearson, 1992.
4. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Purnima Publishing Company, New Delhi, 1997.

**References:**

1. P.M. Silverstein, F.X. Wester, Spectroscopic Identification of Organic Compounds, 6<sup>th</sup> Ed., Wiley 1998.
2. J. Mohan, Organic Spectroscopy Principles and Applications, 2<sup>nd</sup> Ed., CRC, 2004.
3. I.L. Finar, Organic Chemistry, Vol.II, 5<sup>th</sup> ed., ELBS 1975.
4. J. E. Huheey, Inorganic Chemistry, 3<sup>rd</sup> ed., Harper & Row Publishers, Singapore.
5. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, New York, USA.
6. G. L. Eichorn, Inorganic Biochemistry, Volumes 1 & 2, 2<sup>nd</sup> ed., Elsevier Scientific Publishing company, New York, 1973.

**Question Pattern**

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>



Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course					Hours	Credits			
III	20PCH3EC2:2	Selected topics in chemistry – I					6	4			
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)					
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	
CO1	✓		✓	✓	✓		✓	✓	✓	✓	
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
CO3	✓		✓		✓	✓	✓	✓	✓	✓	
CO4	✓		✓		✓	✓	✓	✓		✓	
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓	
Number of Matches(✓) = 42 Relationship: High											

Mapping	1-29%	30-59%	60-69%	70-89%	90-100%
Matches	1-14	15-29	30-34	35-44	45-50
Relationship	Very Poor	Poor	Moderate	High	Very High

## SEMESTER-III

Course Code: 20PCH3EC2:3  
Instruction Hours: 6  
Credits: 4

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### ELECTIVE COURSE 2:3 -AGRICULTURAL CHEMISTRY

#### Course Outcomes

- Students will gain knowledge on concepts and principles of Soil Science
- Understand the role of soil forming factors and processes in soil formation
- Understand various soil physical, chemical and biological properties and their impact on plant growth.
- Imparts knowledge on essential nutrients, soil fertility, nutrient transformations in soil.
- Manures, fertilizers and soil fertility management through various approaches.

#### UNIT- I -Soil Fertility and Soil Productivity(18 – Hours)

Nutrient sources – fertilizers and manures; essential plant nutrients - functions and deficiency symptoms. Soil and fertilizer nitrogen – sources, forms, immobilization and mineralization, nitrification, denitrification; biological nitrogen fixation -types, mechanism, microorganisms and factors affecting; nitrogenous fertilizers and their fate in soils; management of fertilizer nitrogen in lowland and upland conditions for high fertilizer use efficiency.

#### UNIT - II -Fixation Nutrient

(18 – Hours)

Soil and fertilizer phosphorus - forms, immobilization, mineralization, reactions in acid and alkali soils; factors affecting phosphorus availability in soils; phosphatic fertilizers - behavior in soils and management under field conditions, potassium - forms, equilibrium in soils and its agricultural significance; mechanism of potassium fixation; management of potassium fertilizers under field conditions, sulphur - source, forms, fertilizers and their behavior in soils; calcium and magnesium– factors affecting their availability in soils; management of sulphur.

#### UNIT - III- Secondary Macronutrients

(18 – Hours)

Calcium and magnesium fertilizers, micronutrients – critical limits in soils and plants; factors affecting their availability and correction of their deficiencies in plants. Role of chelates in nutrient availability, common soil test methods for fertilizer recommendations; quantity– intensity relationships; soil test crop response correlations and response functions.

#### UNIT - IV-Soil quality

(18 – Hours)

Fertilizer use efficiency; blanket fertilizer recommendations – usefulness and limitations; site- specific nutrient management; plant need based nutrient management; integrated nutrient management, soil fertility evaluation - biological methods, soil, plant and tissue tests; soil quality in relation to sustainable agriculture.

**UNIT - V-Primary Macronutrients****(18 – Hours)**

Chemical analysis of soil for total N,P&K and available nutrients (N, P, K, S, Cu, Fe, Mn,Zn, Mo. B), analysis of plants for essential elements (N, P, K, S, Cu, Fe, Mn, Zn, Mo, B).

**Text Books:**

1. Environmental Chemistry, S. E. Manahan, Lewis Publishers.
2. Environmental Chemistry, Sharma & Kaur, Krishna Pubilshers.
3. Environmental Chemistry, A. K. De, Wiley Easlem
4. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Holler, W. B. Saunders.

**References:**

1. Brady NC & Weil RR. 2002. The Nature and Properties of Soils. 13th Ed. Pearson Edu.
2. Kannaiyan S, Kumar K & Govindarajan K. 2004. BiofertilizersTechnology. Scientific Publ. Leigh JG. 2002. Nitrogen Fixation at the Millennium. Elsevier.
3. Mengel K & Kirkby EA. 1982. Principles of Plant Nutrition. International PotashInstitute, Switzerland.
4. Mortvedt JJ, Shuman LM, Cox FR & Welch RM. 1991. Micronutrients in Agriculture.2nd Ed. SSSA, Madison. Pierzinsky GM, Sims TJ & Vance JF. 2002. Soils andEnvironmental Quality. 2nd Ed. CRC Press.
5. Troeh FR & Thompson LM. 2005. Soils and Soil Fertility. Blackwell.

**Question Pattern**

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course					Hours	Credits			
III	20PCH3EC2:3	Agricultural chemistry					6	4			
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)					
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	
CO1	✓		✓	✓	✓		✓	✓	✓	✓	
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
CO3	✓		✓		✓	✓	✓	✓	✓	✓	
CO4	✓		✓		✓	✓	✓	✓		✓	
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓	
Number of Matches(✓) = 42 Relationship: High											

Mapping	1-29%	30-59%	60-69%	70-89%	90-100%
Matches	1-14	15-29	30-34	35-44	45-50
Relationship	Very Poor	Poor	Moderate	High	Very High

## SEMESTR – III

Course Code: 20PCH3EC3:1  
Instruction Hours: 6  
Credits: 4

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### ELECTIVE COURSE 3:1 - ELECTRO ORGANIC CHEMISTRY

#### Course Outcomes:

- Learn the knowledge about electro organic synthesis and electrochemical reactions
- Learn to the information about cathodic reduction and anodic oxidation reactions
- Learn about the electro organic synthesis.
- Students recognize the different types of electrochemical cells.
- Students are able to recognize and balance oxidation-reduction reactions

#### Describe various Chromatographic techniques **UNIT – I: Basic concepts of electro organic synthesis (18 – Hours)**

Introduction, fundamental aspects of electro transfer reaction : oxidation, reduction reactions vs electron transfer reactions in organic chemistry and electrochemistry - Standard potentials : Mechanism and theory of outer sphere electron transfer reactions – Fundamental aspects of electrode phenomena, monitoring a half-reactions, general view of an electrode reaction, adsorption phenomena – Mass transfer in electro chemistry, fundamental aspects, steady state electrochemical methods, Transient electrochemical methods.

#### **UNIT- II: Methods for studies of electrochemical reactions (18 – Hours)**

Introduction, linear sweep voltammetry and cyclic voltammetry, Experimental setup, simple electrotransfer reaction, electron transfer reaction followed by chemical reaction and solutions, limiting experimental factors – potential step and current step method, chronoamperometry, chronocoulometry, chronopotentiometry – polarography – methods for determination of number of electrons.

#### **UNIT- III: Cathodic reductions (18 – Hours)**

Introduction, formation of radical anions, dianions and polyanions, experimental aspects, thermodynamics kinetics, addition of electrophilic reagents and related reaction, dimerization. Electrochemical reduction of halogenated compounds: monohalogenated alkanes, halogenated aromatic compounds, acyl halides, aliphatic alpha – halo carbonyl compounds, cathodic reduction of nitro and related compounds, Aliphatic nitro compounds, aromatic nitro compounds (preparation of para amino phenol nitrobenzenes, nitramines and azides). Electrochemical reduction of carbonyl compounds, general aspects.

#### **UNIT- IV: Anodic oxidation of organic compounds (18 – Hours)**

Introduction, general mechanistic consideration, direct anodic oxidation, indirect anodic oxidation. Anodic oxidation of hydrocarbons, nitrogen containing compounds. Electrosynthesis of Bioactive materials: Introduction, simple Kolbe oxidation: application to synthesis of (+) -  $\alpha$  onxerin and (+) – penta cyclosqualene, Kolbe cyclisation and Tandem cyclization.

**UNIT- V: Special topic in electro organic synthesis****(18 – Hours)**

Paired electro organic synthesis, simple examples – electrogenerated reagents  
 Homogeneous redox catalysts – General aspects of indirect electron exchanges, pure redox catalysis (general case) – use of indirect electrochemical reactions in synthesis, oxidations, reductions – Electrogenerated superoxides. Electrochemical partial fluorination: Introduction, Anodic fluorination of aromatic compounds, olefins, carbonyl compounds, heterocyclic compounds. Electro enzymatics synthesis: Introduction, principles of redox catalytic enzyme activation and co-factor regeneration – electroenzymatic reductions and oxidation (simple examples only).

**References:**

1. Organic electro chemistry by Henning Lund & Ole Hammerich, 4th edition, Publisher: Marcel Dekker, Inc, New York.

**Question Pattern**

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
III	20PCH3EC3:1	Electro organic chemistry	6	4						
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓		✓	✓	✓		✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO3	✓		✓		✓	✓	✓	✓	✓	✓
CO4	✓		✓		✓	✓	✓	✓		✓
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER – III

Course Code: 20PCH3EC3:2  
Instruction Hours: 6  
Credits: 4

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### ELECTIVE COURSE 3:2 - ANALYTICAL CHEMISTRY

#### Course Outcomes:

- Learn to instrumental methods
- Learn the nature of errors and their types.
- Learn the various techniques in chromatography.
- The course make the student to learn how to prepare solutions quantitatively and analysis the analyze with high accuracy.
- Describe various Chromatographic techniques

#### UNIT I: Analytical Techniques

(18 – Hours)

**Analytical chemistry** - chemical analysis – Advantages and limitations of chemical methods- types of chemical analysis- Instrumental methods- Advantages and Limitations of Instrumental methods- Analytical methods on the basis of Sample size – Sampling- sampling methods- sampling in different physical states- Sampling statistics- source of error in sampling- dangers during sampling.

**Techniques of Analysis** – Introduction- Classification of analytical techniques- classification of instrumental methods of analysis - factors affecting the choice of analytical methods- interferences- typical separation procedures- sensitivity and detection limits.

#### UNIT –II Data Analysis

(18 – Hours)

Mean, Average, Standard Deviation, Variance and its testing– Correlation and Regression – Least square method for curve fitting.

#### UNIT III: Chromatography

(18 – Hours)

Solvent extraction – principles of ion exchange, paper, thin-layer and column chromatography techniques – columns, adsorbents, methods, R<sub>f</sub> values, McReynold's constants and their uses – HPTLC, HPLC techniques – adsorbents, columns, detection methods, estimations, preparative column – GC-MS techniques – methods, principles and uses.

#### UNIT IV: Thermoanalytical Methods and Fluorescence Spectroscopy (18 – Hours)

Principles – instrumentations and applications of thermogravimetry analysis (TGA), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC) – thermometric titrations – types – advantages. Basic aspects of synchronous fluorescence spectroscopy – spectral hole burning – flow cytometry – fluorometers (quantization) – instrumentation – applications.

**UNIT V: Electroanalytical Techniques****(18 – Hours)**

Electrochemical sensors, ion-sensitive electrodes, glass – membrane electrodes, solid-liquid membrane electrodes – ion-selective field effect transistors (ISFETs) – sensors for the analysis of gases in solution.

Principles and applications of extended X-ray absorption fine structure (EXAFS) – surface extended X-ray absorption (SEXAFS) – atomic absorption spectroscopy (AAS) – flame emission spectroscopy (FES) – turbidimetry – theory and applications.

**Text Books:**

1. H. Kaur - “Instrumental methods of Chemical Analysis”, 6th edition, (2010), Pragati prakasan Publications, Meerut.
2. H. H. Willard, L. L. Merritt, J. A. Dean and F. A. Settle, Instrumental Methods of Analysis; 6th Ed., CBS Publishers and Distributors, Chennai, 1986.
3. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy; 4<sup>th</sup> Ed., Tata McGraw-Hill, New Delhi, 1994.
4. I. Vogel, Text Book of Quantitative Inorganic Analysis; 6th Ed., Longman, New Delhi, 2000.
5. S. C. Gupta, Fundamentals of Statistics; 6th Ed., Himalaya Publications, Delhi, 2006

**References:**

1. D. B. Hibbert and J. J. Gooding, Data Analysis for Chemistry; Oxford University Press, UK, 2006.
2. J. Topping, Errors of Observation and Their Treatment; 4th Ed., Chapman Hall, London, 1984.
3. Braithwaite and J. F. Smith, Chromatographic Methods; 5th Ed., Springer, Germany; 1995.
4. K. Srivastava and K. K. Srivastava, Introduction to Chromatography; 2nd Ed., Holden Day, New York, 1985.
5. D. A. Skoog, D. M. West and D. J. Holler, Fundamentals of Analytical Chemistry, 7th Ed., Harcourt College Publishers, Singapore, 2004.
6. Sharma, S. G. Schulman, Introduction to Fluorescence Spectroscopy; Wiley-Interscience, New York, 1999.
7. D. C. Harris, Quantitative Chemical Analysis; 4th Ed., W. H. Freeman Publications, New York, 1995.

**Question Pattern**

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>



Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course					Hours	Credits			
III	20PCH3EC3:2	Analytical chemistry					6	4			
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)					
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	
CO1	✓		✓	✓	✓		✓	✓	✓	✓	
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
CO3	✓		✓		✓	✓	✓	✓	✓	✓	
CO4	✓		✓		✓	✓	✓	✓		✓	
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓	
Number of Matches(✓) = 42 Relationship: High											

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER – III

Course Code: 20PCH3EC3:3  
Instruction Hours: 6  
Credits: 4

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### ELECTIVE COURSE 3:3 - MEDICINAL CHEMISTRY

#### Course Outcomes:

After completing the course, students shall be able to:

- Describe the various stages involved in the development of a drug,
- Describe the "interaction between ligand and receptor" concept
- Describe methods for medicinal chemistry, including combinatorial chemistry,
- Actively participate in discussions during seminars and group exercises
- Application the gained knowledge about the therapeutic classes of drugs.

#### UNIT-I -Molecular Basis Of Drug Action (18 – Hours)

Receptor: Drug Receptor Interaction. Basic ligand concept, agonist, antagonist, partial agonist, inverse agonist. Receptor Theories - Occupancy, Rate & Activation Theories. Receptor Binding Assays, Determination of B-max and Kd by transforming data with Hill plot and Scatcherd plot. Above concepts with special reference to Opioid, Histaminergic, Adrenergic and GABA nergic receptors. Enzyme Inhibitors as drugs - ACE, leukotrienes, Lipoxygenase, Cyclooxygenase. DNA Polymerase Inhibitors, HIV - Protease / Reverse Transcriptase, Integrase and Cytochrome P-450 Inhibitors. Drug binding to nucleic acid -- Antimalarial, anti-cancer, antiviral

#### UNIT-II - Drug Design (18 – Hours)

Design And Application Of Prodrugs –Prodrug concept. Prodrugs of various functional groups like carbonyl, hydroxy. amide, amines. Application of Prodrug approach to-Improvement of bioavailability -Prevent first pass metabolism. Reduction of side effects-Prolong duration of action-Site specific delivery

#### UNIT-III- Antibiotics (18 – Hours)

Historical background, Nomenclature, Stereochemistry, Structure activity relationship, Chemical degradation classification and important products of the following classes.

**β-Lactam antibiotics:** Penicillin, Cephalosporins, β- Lactamase inhibitors, Monobactams  
**Aminoglycosides:** Streptomycin, Neomycin, Kanamycin Tetracyclines: Tetracycline, Oxytetracycline, Chlortetracycline, Minocycline, Doxycyclin.

#### UNIT – IV -Introduction to Drug Design (18 – Hours)

Various approaches used in drug design. Physicochemical parameters used in quantitative structure activity relationship (QSAR) such as partition coefficient, Hammett's electronic parameter, Taft's steric parameter and Hansch analysis. Pharmacophore modeling and docking techniques.

**Combinatorial Chemistry:** Concept and applications chemistry: solid phase and solution phase synthesis. of combinatorial

**UNIT – V-Principle of drug design****(18 – Hours)**

Analogue synthesis versus rational design; discovery of lead compounds, Pharmacophoric identification, Prodrugs and soft drug. Ring Analogues of Phenothiazines: Chlorprothixene, Thiothixene, Loxapine succinate, Clozapine. Fluro buterophenones: Haloperidol, Droperidol, Risperidone. Beta amino ketones: Molindone hydrochloride. Benzamides: Sulpieride.

**Recommended Books**

1. Burger: Medicinal Chemistry (John Wiley & Sons N.Y.)
2. Foe: Principles of Medicinal Chemistry (Varghese & Co.)
3. Text Book of Bio-chemistry
4. Molecular biology - Walson & Crick

**Reference Books:**

1. Lednicer: Organic Drug synthesis Vol. 1, 2, 3, 4 (John Wiley & Sons N.Y.)
2. Bunerworther Progress in Medicinal Chemistry Series
3. Wilson & Gisvold - Text book of Medicinal Chemistry (J.B. Lippincoff cam)
4. Stuart Warren: Organic Synthesis- The Disconnection, approach (John Wiley)

**Question Pattern**

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
III	20PCH3EC3:3	Medicinal Chemistry	6	4						
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓		✓	✓	✓		✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO3	✓		✓		✓	✓	✓	✓	✓	✓
CO4	✓		✓		✓	✓	✓	✓		✓
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

Mapping	1-29%	30-59%	60-69%	70-89%	90-100%
Matches	1-14	15-29	30-34	35-44	45-50
Relationship	Very Poor	Poor	Moderate	High	Very High

## SEMESTER – III

Course Code: 20PCH3CP5

Instruction Hours: 6

Credits: 4

Exam Hours: 6

Internal Marks: 40

External Marks: 60

### CORE COURSE PRACTICAL - 5 - PHYSICAL CHEMISTRY NON-ELECTRICAL PRACTICAL

#### Course Outcomes:

- Learn the chemical kinetics.
- Learn the adsorption techniques using Freundlich isotherm
- Learn the Phase diagram
- Learn the polymerization.
- Learn to calculate molecular weight.

#### Any ten experiments from the following experiments (to be decided by the course teacher):

1. Kinetics – Acid Hydrolysis of Ester – Comparison of strength of acids.
2. Kinetics – Acid Hydrolysis of Ester – Determination of Energy of Activation ( $E_a$ ).
3. Kinetics – Saponification of Ester – Determination of  $E_a$  by conductometry.
4. Kinetics–Persulphate–Iodide Reaction–Determination of order, effect of Ionic strength on rate constant.
5. Polymerization – Rate of polymerization of acrylamide.
6. Distribution Law – Study of iodine – Iodide equilibrium.
7. Distribution Law – Study of Association of Benzoic Acid in Benzene.
8. Adsorption – oxalic Acid/Acetic Acid on charcoal using Freundlich isotherm.
9. Determination of critical solution temperature of phenol-water system and effect of impurity of added electrolyte on CST.
10. Determination of molecular weight by Rast Macro method
11. Determination of molecular weight by Transition Temperature.
12. Determination of eutectic temperature and eutectic composition of binary mixture.
13. Determination of primary salt effect.

#### References:

1. Daniels, I., Experimental Physical Chemistry, (7th edition), New York, McGraw Hill, (1970).
2. B.P. Levitt, Ed., Findlay's practical Physical Chemistry, 9<sup>th</sup> Ed., Longman, 1985.
3. J.N. Gurtu, R. Kapoor, Advanced Experimental Chemistry, Vol. I, S.Chand & Co., 1987.

### Scheme of valuation

Criteria	Marks
Record	5
Aim and tabulation	10
Calculation	10
Results	35
Allowed error 5%	20
5-10%	10
10%<	

### Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
III	20PCH3CP5	Physical chemistry non-electrical practical	6	4						
<b>Course Outcomes (COs)</b>	<b>Programme Outcomes(POs)</b>					<b>Programme Specific Outcomes(PSOs)</b>				
	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PSO1</b>	<b>PSO2</b>	<b>PSO3</b>	<b>PSO4</b>	<b>PSO5</b>
<b>CO1</b>	✓		✓	✓	✓		✓	✓	✓	✓
<b>CO2</b>	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
<b>CO3</b>	✓		✓		✓	✓	✓	✓	✓	✓
<b>CO4</b>	✓		✓		✓	✓	✓	✓		✓
<b>CO5</b>	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER – IV

Course Code: 20PCH4CC8  
Instruction Hours: 6  
Credits: 4

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### CORE COURSE – 8 - ELECTROCHEMISTRY, SURFACE PHENOMENA AND STATISTICAL THERMODYNAMICS

#### Course Outcomes:

- Learn improve the quantum chemistry and electrochemistry.
- Learn the detailed information about thermodynamics.
- Learn the surface phenomena.
- To learn the group theory.
- Learn the symmetry of elements.

#### UNIT- I: Applications of Group Theory

(18 – Hours)

Applications of Group Theory- The Direct Product and its Applications, Applications of Group theory to Spectroscopy – Vanishing of Integrals, Symmetry selection rules for Vibrational, Raman and electronic spectroscopy. Infra red Spectroscopy – Reduction Formula – Determination of Normal Modes of Vibration and IR activity for H<sub>2</sub>O and NH<sub>3</sub> Molecule, Vibrational Raman Spectroscopy for H<sub>2</sub>O and NH<sub>3</sub> Molecule, Electronic Spectra of Formaldehyde. Hybridization Schemes of Orbitals (sp<sup>3</sup>, sp<sup>2</sup>, dsp<sup>2</sup>, sp<sup>3</sup>d<sup>2</sup>), Projection Operator – Symmetry Adapted Linear Combination (SALC) Procedure. Symmetry factoring of secular determinant and its applications to butadiene.

#### UNIT-II: Electrochemistry-I

(18 – Hours)

Ionics: Debye-Huckel theory - radius of ionic atmosphere and its calculation – Debye-Huckel-Onsager equation and its modifications - asymmetry and electrophoretic effects – Debye Falkenhagen and Wien's effects - Activity of ions in solutions - Debye Huckel limiting Law. Electrode - electrolyte equilibrium: Nernst equation derivation and its limitations - equilibrium electrode potentials - Calomel electrode, concentration cells - liquid junction potentials - Thermodynamic quantities from EMF data.

#### UNIT- III: Electrochemistry-II

(18 – Hours)

Electro kinetic Phenomena: Theories of electrical double layer - Theory of multiple layers at electrode electrolyte interface - electro kinetic phenomena. Processes at electrodes - the rate of charge transfer - current density – Butler-Volmer equation - Taft equation. Principles and applications of Polarography - Instrumentation, Types of cells, advantages of dropping mercury electrode, interpretation of current voltage curves, determination of 'n' value, polarographic maxima. Cyclic voltammetry, advantages over polarography

techniques - test of reversibility of electron transfer reactions. Corrosion and passivation of metals - Pourbaix diagram - Evans diagram - Batteries and Fuel cells - Ion selective electrodes.

#### **UNIT - IV : Surface Phenomena**

**(18 – Hours)**

B.E.T. isotherms - Surface area determination - Adsorption, adsorbent, adsorbate, physisorption, chemisorptions and van der Waals forces. Heat of adsorption and its determination - Adsorption from solution, Gibbs adsorption isotherm - solid - liquid interfaces - wetting and contact angle - solid gas interfaces - soluble and insoluble film. Surface tension - methods of measuring surface tension - electrical phenomenon at Interfaces, including electro kinetic, micelles and reverse micelles, Solubilisation, Micro-emulsions. Role of surface in catalysis - semiconductor catalysis, n and p type surfaces - kinetics of surface reactions involving adsorbed species - Langmuir - Hinshelwood mechanism.

#### **UNIT - V : Statistical Thermodynamics**

**(18 – Hours)**

Partition functions: Translational, rotational, vibrational, electronic - calculation of enthalpy, internal energy, entropy and other thermodynamic functions - application of partition functions to mono and diatomic molecules. Heat capacity of solids: Einstein and Debye's treatments - concept of negative Kelvin temperature. Non-equilibrium thermodynamics: Thermodynamics of irreversible process - enthalpy production and entropy flow in open system - Onsager theory - phenomenological relations - Onsager reciprocal relations - steady state conditions.

#### **Text Books:**

1. K.V.Raman Group theory and its Application to Chemistry. Tata McGraw - Hill Pu Samuel Glasstone - Textbook of Physical Chemistry 5th Ed. 2010, MacMillan India.
2. F. A. Cotton, "Chemical Application of Group Theory", 2nd edition, Wiley - Eastern Press, 1995.

#### **References:**

1. H. Goldstein, Classical Mechanics, Addison - Wesley Publishing company, 1956.
2. S. Glasstone, Introduction to Electrochemistry, Affiliated East-West Press, 1968.
3. D. R. Crow, Electrochemistry, Academic Press, New York
4. D. R. Crow, Polarography of metal complexes, Academic Press, New York
5. Daniel C. Harris, Quantitative Chemical Analysis, 4th edn, W.H. Freeman and Company, New York, 1995
6. P.W. Atkins - Physical Chemistry E.L.B.S. 6th Ed. 1998.
7. K.L. Kapoor - A text book of physical chemistry, Macmillan India press, Chennai - 2009.
8. P. W. Atkins, Physical Chemistry, ELBS and Oxford University Press, Oxford, 1983
9. J. Rajaram and J. C. Kuriacose, Thermodynamics for students of Chemistry - Classical, Statistical and Irreversible, Shobhan Lal Nagin, New Delhi, 1981



### Question Pattern

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
<b>IV</b>	20PCH4CC8	Electrochemistry, surface phenomena and statistical thermodynamics	6	4						
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
<b>CO1</b>	✓		✓	✓	✓		✓	✓	✓	✓
<b>CO2</b>	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
<b>CO3</b>	✓		✓		✓	✓	✓	✓	✓	✓
<b>CO4</b>	✓		✓		✓	✓	✓	✓		✓
<b>CO5</b>	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

Mapping	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER – IV

Course Code: 20PCH4EC4:1

Instruction Hours: 6

Credits: 4

Exam Hours: 3

Internal Marks: 25

External Marks: 75

### ELECTIVE COURSE 4:1 - INSTRUMENTATION TECHNIQUES

#### Course Outcomes:

- Learn improve the technical knowledge about various spectroscopy.
- Learn the detailed information about conductometry.
- Learn the separation of compounds by using chromatography.
- Learn the ion fragmentation.
- Learn the prediction of NMR.

#### UNIT-I : UV- Visible spectroscopy

(18 – Hours)

Instrumentation- sources, filters and monochromators, slits, grating, cuvette, radiation detectors and indicators, photoelectric spectrophotometer - types, sources of errors during recording, calibration- presentation of spectral data Infrared Spectroscopy: Dispersive infrared spectrometer- source (Nernst, Globar) monochromator, detector, double-beam spectrophotometer - presentation of spectra- sample preparation techniques for IR, FT-IR- simple diagram of a Fourier transform infrared spectrometer- working mode – advantages. Raman spectroscopy: Instrumentation- source of light, filters, sample holders, spectrograph, detectors, Sample preparation.

#### UNIT-II: Nuclear Magnetic Resonance (NMR)

(18 – Hours)

Instrumentation - magnet, magnetic field sweep, radio frequency source, signal detector and recording system, sample holder, sample probe. Electron Spin Resonance (ESR): Instrumentation - electromagnet, source of micro wave radiation, sample cavity, choice of solvent, crystal detectors and recorder-double resonance spectrometers. Mass Spectrometry: Instrumentation - sample preparation, generation of ions, analyzer, ion collector and measuring system, resolution- representation of mass spectrum – double focusing mass spectrometer.

#### UNIT-III: Conductometry

(18 – Hours)

Introduction, laws and definitions of conductance, effects of dilution, conductance measurements, conductometric titrations - apparatus, types and advantages. Potentiometry: electrochemical series, reference electrodes – hydrogen electrode, calomel and silver-silver chloride electrode, measurement of pH – glass indicating electrode, potentiometric titrations, variations in potentiometric titrations, its advantages. Atomic Absorption Spectroscopy: Introduction, principle of AAS, classification of atomic spectroscopic methods, measurement of atomic absorption, instrumentation – application. Atomic **Emission spectroscopy** – Introduction, origin of spectra, principle of emission spectroscopy, Instrumentation, measurement of light intensity and applications.

**UNIT-IV: Ion Chromatography****(18 – Hours)**

Electrophoresis : Separation by Adsorption- Affinity techniques, Affinity elution from Ion exchangers and other Adsorbents, Pseudo affinity adsorbents polycrylamide gel electrophoresis, Isoelectric focussing Isotachopheresis, Two dimensional gel electrophoresis, Capillary electrophoresis in rotation- stabilized media, Electrophoresis in stabilized salts. Applications in Nuclei acids, Clinical and capillary zone electrophoresis of carbohydrates.

**UNIT-V: Mass Spectroscopy****(18 – Hours)**

Mass spectrometry principle, Instrumentation, Ionization methods – EL, CI, FAB, arc & spark, photoionization, thermal ionization, FI\*& FD, laser induced, Photoelectric ionization, SIMS, Mass analyzers – Magnetic, Double focussing, Time of flight, Quadrupolar, Ion cyclotron resonance analyzer. Coupled techniques, GC FTIR, GCMS (Use of stable isotopes) HPLC-MS.

**Text Books:**

1. H. Kaur - “Instrumental methods of Chemical Analysis”, 6th edition, (2010), Pragati prakasan Publications, Meerut.
2. B.K. Sharma – “Instrumental methods of Analysis”, (2000), Goel Publications.
3. R.A. Day and A.L. Underwood – “Quantitative Analysis”, (1999), Prentice-Hall of India Pvt., Ltd., New Delhi.

**References:**

1. Willard, Meritt, Dean and Settle – “Instrumental Methods of Analysis”, 7th Ed.,(2006), CBS Publishers.
2. S.M. Khopkar, “Basic Concepts of Analytical Chemistry”, Revised edition (2006) Wiley Eastern Ltd.
3. B.S. Furniss, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell – “Vogel’s Text book of Practical Organic Chemistry”, fifth edition ,2009, Pearson Education Publisher.
4. L.Pavia – “Spectroscopy” cengage CourseIndia Pvt. Ltd – 2010.
5. Harald Guther, “NMR Spectroscopy”, Wiley india (p) Ltd, 2nd Edn,2010.
6. G.Aruldas –“Molecular structure & Spectroscopy ”,PHI CoursePvt.Ltd.2nd Edition , - 2008.
7. Colin N.Banwell – “Fundamentals of Molecular structure Spectroscopy ” Mc.Grow – Hill publishing company Ltd. 4th edition ,,1995.

**Question Pattern**

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course					Hours	Credits			
IV	20PCH4EC4:1	Instrumentation techniques					6	4			
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)					
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	
CO1	✓		✓	✓	✓		✓	✓	✓	✓	
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
CO3	✓		✓		✓	✓	✓	✓	✓	✓	
CO4	✓		✓		✓	✓	✓	✓		✓	
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓	
Number of Matches(✓) = 42 Relationship: High											

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER-IV

Course Code: 20PCH4EC4:2  
Instruction Hours: 6  
Credits: 4

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### ELECTIVE COURSE 4:2 - NANO AND GREEN CHEMISTRY

#### Course Outcomes:

- Learn a basic idea on nano and green chemistry
- Learn the knowledge about solvent free reactions
- Learn about the sono chemistry.
- Learn the various spectroscopies.
- Learn the essentials of green chemistry.

#### UNIT - I: Synthesis And Applications Of Nanomaterials (18 Hours)

Preparation of nanomaterials – plasma arcing, CVD, electrodeposition, sol-gel synthesis, ball milling, uses of natural nano particles. Synthesis and applications of carbon nanotubes. Self assembled mono layers – mono layers on gold – preparation – structure – growth process – patterning mono layers – mixed mono layers.

Semiconductor quantum dots – synthesis – electronic structure & spectral properties  
Monolayer-protected metal nano particles – characterization – functionalization–

Application - Core-Shell nano particles – introduction – types of systems – characterization – properties – Applications of Nanosensors – electrochemical sensors, sensors based on physical properties – nanobiosensors.

#### UNIT - II: Characterization Of Nanomaterials (18 Hours)

Electron microscopes – scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Scanning Transmission Electron Microscopy (STEM), Scanning Probe Microscopy (SPM) – scanning tunneling microscopy (STM) – Atomic manipulations, Focused Ion beam (FIB) technique – Atomic force microscopy (AFM) – scanning probe Lithography (SPL), Dip pen nanolithography (DPN) - Optical microscopies for nanoscience and Technology – Confocal microscopy – scanning near-field optical microscopy – particle size analysis.

#### UNIT-III: Carbon nanotubes (18 Hours)

CNT –definition- Classification –Single wall CNT- Multiwall CNT- Preparation - arc method –laser ablation method – Chemical vapour deposition method – Electro-deposition method- Ball milling method. SWCNT and MWCNT – Properties- applications – fullerenes – properties – uses. Nanocomposites – Classification – Properties - uses.

**UNIT-IV: Essentials Of Green Chemistry****(18 Hours)**

Introduction to green chemistry-definition, origin, history, needs, goals, twelve principles of green chemistry. Usage of Conventional and Green solvents-Advantages, Limitations and drawbacks. Green Synthesis – Designing, Choice of starting materials, choice of reagents, choice of catalysts: bio catalysts, polymer supported catalysts, choice of solvents. Synthesis involving basic principles of green chemistry. Examples: synthesis of adipic acid, methyl methacrylate, paracetamol. Microwave, Ultrasonication and Ultrasound assisted reactions – esterification, reduction AND coupling reactions.

**UNIT-V: Green Synthesis****(18 Hours)**

Adipic acid – catechol- methyl methacrylate, acetaldehyde, Ibuprofen, Paracetamol- Microwave assisted reaction in water- Definition – Hofmann eliminations – Hydrolysis- Oxidation- Microwave assisted reaction in organic solvents- Esterification – Fries rearrangement – Decarboxylation- Diels – Alder reaction. Ultrasound assisted reaction: Definition- Cannizaro reaction – Strecker synthesis – Reformatsky reaction.

**Text Books:**

1. Sulabha K. Kulkarni Nanotechnology: Principles and practices (capital Pvt. Co.)-2002.
2. R.Sanghi and M.M srivastva, Green chemistry, Narosa P ublications, 2003.

**References:**

1. Nanoscale materials in chemistry, Wiley interscience, Kenneth, J.Klaburde, 2002.
2. M. M. Srivastva and R.Sanghi, Chemistry for green environment, Narosa, 2005.
3. S, Delvin Green chemistry, IVY publication house, 2006.
4. F.J. Ownes Introduction to Nano technology John Wiley and New Jersey, 2003.

**Question Pattern**

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course					Hours	Credits			
IV	20PCH4EC4:2	Nano and green chemistry					6	4			
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)					
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	
CO1	✓		✓	✓	✓		✓	✓	✓	✓	
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
CO3	✓		✓		✓	✓	✓	✓	✓	✓	
CO4	✓		✓		✓	✓	✓	✓		✓	
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓	
Number of Matches(✓) = 42 Relationship: High											

Mapping	1-29%	30-59%	60-69%	70-89%	90-100%
Matches	1-14	15-29	30-34	35-44	45-50
Relationship	Very Poor	Poor	Moderate	High	Very High

## SEMESTER – IV

Course Code: 20PCH4EC4:3  
Instruction Hours: 6  
Credits: 4

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### ELECTIVE COURSE 4:3 - INORGANIC AND ORGANIC PHOTOCHEMISTRY

#### Course Outcomes:

- Understand the concepts related to light induced organic synthesis, mechanisms and the functions of various reagents.
- Apply their understanding about the photochemical reactions of industrial significance.
- Analyze the product distribution and the stereochemistry of various organic products derived from photochemistry.
- Evaluate the photochemical reactions based on the influence of the substituents on substrate molecules.
- Design new photochemical reactions in order to achieve the required product(s).

#### UNIT-I Metal Complexes Spectra

(18 Hours)

Excited States of Metal Complexes-Excited states of metal complexes: comparison with organic compounds, electronically excited states of metal complexes, charge-transfer spectra, charge transfer excitations, methods for obtaining charge-transfer spectra.

#### UNIT-II Photochemistry Reaction

(18 Hours)

Ligand Field Photochemistry-Photosubstitution, photooxidation and photoreduction, lability and selectivity, zero vibrational levels of ground state and excited state, energy content of excited state, zero zero spectroscopic energy, development of the equations for redox potentials of the excited states.

#### UNIT-III Inorganic Photochemistry

(18 Hours)

Inorganic Photochemistry : Basic principles, Basic photochemical processes, Kasha's rule, Thexi state, Photochemical behaviour of transition metal complexes, charge transfer spectra of crystalline and gaseous alkali halides, photochemical reactions of coordination compounds, oxidation-reduction reactions, Photo substitution reactions, Adamson's rules and photosubstitution reactions of cobalt(III) complexes i.e.  $[\text{Co}(\text{NH}_3)_5\text{X}]^{2+}$ ,  $[\text{Co}(\text{en})_3]^{3+}$ , and chromium(III) complexes i.e.  $[\text{Cr}(\text{H}_2\text{O})_6]^{3+}$  and  $[\text{Cr}(\text{NH}_3)_6]^{3+}$  and ruthenium (II) polypyridyl complexes.

#### UNIT-IV Organic Photochemistry

(18 Hours)

Organic Photochemistry: Photochemical energy plank Condon Principle, Jablonski diagram singlet and triplet states, dissipation of photochemical energy, photosensitization, quenching, quantum efficiency and quantum yield, experimental methods of



photochemistry. transitions Norrish type I and Norrish  $\pi=\pi$ ,  $\pi$ -Photochemistry of carbonyl compounds- n type II cleavages, patterno-Buchi reaction.

### UNIT-VRearrangement

(18 Hours)

Photoreduction photochemistry of enone - Hydrogen abstraction, rearrangement of  $\alpha$  -  $\beta$  - unsaturated ketones and cyclohexadienes, Photochemistry of p- Benzoquinones, photochemistry of unsaturated systems - Olefins, cis trans Isomerisation and dimerization hydrogen abstractions and, addition acetylenes dimerisation, dienes - Photochemistry of 1,3 butadienes (2+2) additions leading to cage structures photochemistry .of cyclohexadienes.

#### Text books:

- 1.Introduction to Inorganic Photochemistry, Arjun Singh Negi, Cyber Tech Publication, New Delhi.
2. Inorganic Photochemistry, Fmiza Hammer, Sarup Book Publishers Pvt. Ltd., New Delhi.
3. Concepts of Inorganic photochemistry, A. W. Adamson and P D Fleischaves Wiley.
4. Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March, Me.Graw Hill and Kogakush.
- 5.Molecular reactions and Photochemistry by Charles Dupey and O. Chapman, Prentice Hall.

#### Reference:

1. Mechanisms and Theory in Organic Chemistry by T.H. Lowery and K.S. Richardson.
2. The modern structural theory in Organic Chemistry by L.N.Ferguson, Prentice Hall
3. Physical Organic Chemistry by Jack Hine, Mc. Graw Hill.
- 4.Advanced Inorganic Chemistry- Cotton and Wilkinson
5. Inorganic Chemistry- T.Moeller

#### Question Pattern

Section :A (1 Marks)	MCQ Type	20x1=20
Section :B (5 Marks)	Either OR choice	5x5=25
Section :C (10 Marks)	Answer three out of five	3x10=30
Total Marks		75

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course					Hours	Credits			
IV	20PCH4EC4:3	Inorganic and organic photochemistry					6	4			
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)					
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	
CO1	✓		✓	✓	✓		✓	✓	✓	✓	
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
CO3	✓		✓		✓	✓	✓	✓	✓	✓	
CO4	✓		✓		✓	✓	✓	✓		✓	
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓	
Number of Matches(✓) = 42 Relationship: High											

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER – IV

Course Code: 20PCH4EC5:1

Instruction Hours: 6

Credits: 5

Exam Hours: 3

Internal Marks: 25

External Marks: 75

### ELECTIVE COURSE 5:1 - INDUSTRIAL CHEMISTRY

#### Course Outcomes:

- Learn develop the knowledge about chemical industries
- Learn the fuels and dyes
- Learn about synthesis of dyes and polymer chemistry
- Learn the application of chemistry in quality control measurements.
  
- Learn about the polymers.

#### UNIT-I: Green Methods and Industrial Process (18 – Hours)

Basic ideas about unit operation – Flow charts – Chemical conversion – Batch versus continuous processing – Chemical process selection – Design – Chemical process control- Research & Development and its role in chemical industries. Industrial safety measures – Fire extinguisher, Fire retardant materials – Fire retarding wood – Procedures for handling toxic chemicals

#### UNIT-II: Renewable Energy Resources (18 – Hours)

Renewable energy sources: types of renewable energy sources. Solar cells: basic principles, types and their applications. Fuel cells: basic principles, types and their applications. Working principle and applications of Biofuel cells-brief introduction about hydroelectric, biomass, wind power and geothermal power and their applications and limitations-energy from some other natural source.

#### UNIT III: Polymers(18 – Hours)

Polymers - definition - types of polymers - liquid crystalline polymers. Molecular mass - number and mass average molecular mass - determination of molecular mass (osmometry, viscosity, diffusion, light scattering, and sedimentation methods). viscoelasticity, Rubber elasticity. Kinetics of linear stepwise polymerization - addition polymerization - free radical, cationic and anionic polymerization. Kinetics of copolymerization. Polymerization in homogeneous and heterogeneous systems - stereochemistry and mechanism of polymerization. Coordination Polymerization: Kinetics; mono and bimetallic mechanism.

#### UNIT IV: Commercial Polymers (18 – Hours)

Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers-Fire retarding polymers and electrically conducting polymers. Biomedical polymers.

**UNIT-V: Industrial Water Pollution and its Control & Analysis (18 – Hours)**

Sources of water pollution – domestic – industrial – agricultural – soil and radioactive wastes as sources of pollution. Water pollutants and their effects. Objectives of analysis – parameter for analysis-colour – turbidity – total solids – conductivity – acidity – alkalinity – hardness –chloride – sulphate – fluoride – silica – phosphates, different forms of nitrogen, DO, BOD, COD Heavy metal pollution-public health significance of Cadmium – Chromium – Copper – Lead – Zinc – Manganese. Prevention and control its measures.

**Text Books:**

1. B. K. Sharma, Industrial Chemistry; 8th Ed., Goel Publishing House, New Delhi, 1997.
2. V.R.Gowariker, N.V. Viswanathan and Jayadev Sreedhar, Polymer Science, New Age Publishers, New Delhi, 1986.
3. B.K. Sharma and H. Kaur, “Environmental chemistry” ,Goel Publishing House, Meerut, 2008

**References:**

1. Chemical Process Industries – Norrish Shreve, R. and Joseph A. Brink Jr. McGraw Hill, Industrial Book Company, London.
2. Production and Properties of Industrial Chemicals – Brain A.C.S. Reinhold – New York.
3. Petroleum Products Hand Book. Guthrie V., McGraw Hill, Tokyo.
4. Outlines of Chemical Technology – For the 21st Century – M. Gopala Rao & Matshall Sittig (3rd Edition)
5. Charles E. Carraher, Polymer chemistry, 6th edn, Marcel Dckker, Pvt .Ltd, 2003.
6. F.W.Billmeyer, Jr., A Text Book of Polymer Science, Wiley & Sons, New York, 1971.

**Question Pattern**

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course					Hours	Credits			
IV	20PCH4EC5:1	Industrial chemistry					6	5			
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)					
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5	
CO1	✓		✓	✓	✓		✓	✓	✓	✓	
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
CO3	✓		✓		✓	✓	✓	✓	✓	✓	
CO4	✓		✓		✓	✓	✓	✓		✓	
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓	
Number of Matches(✓) = 42 Relationship: High											

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High

## SEMESTER – IV

Course Code: 20PCH4EC5:2  
Instruction Hours: 6  
Credits: 4

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### ELECTIVE COURSE 5:2 - POLYMER CHEMISTRY

#### Course Outcomes:

- Learn the knowledge in Polymer Chemistry
- Use essential descriptions about polymer chemistry.
- Defines related concepts.
- Different kind of polymers and their properties
- An understanding of basic principles of design and color, concepts, media and formats and the ability to apply them to a specific aesthetic intent.

#### Unit-I

(18 – Hours)

**Industrial Polymers** - Basic Concepts of Polymers-History-Trends and General Polymer Background-Concept of functionality and reactivity-Degree of polymerization. Techniques of Polymerization - Bulk-Solution - Emulsion - Suspension and Interfacial polymerization.

**Classification of Polymers:** Homopolymers-co-polymers-linear polymers-branched polymers-cross linked or three dimensional polymers-block co-polymers-organic-inorganic polymers-natural and synthetic polymers-chain and step growth polymers-thermoplastic and thermoset-based on applications- fibers-foams-adhesives and elastomers-based on performance-commodity and engineering polymers.

#### Unit- II

(18 – Hours)

**Identification of Polymers:** Preliminary tests-Elemental analysis-solubility chart-Specific end group analysis (Acid value-Hydroxyl Value-Iodine value-Epoxy value-SAP Value-Amine value) Spectroscopic analysis (IR & NMR). Solubility chart for identification of polymers-Specific chemical tests for various polymers and group analysis.

#### Unit- III

(18 – Hours)

**Paint Technology** Paints-Introduction and Definitions of paints-pigments-varnishes-lacquers, Anatomy of paints-functions & requirements of constituents of paints-classification of paints on the basis of order of application-methods of curing-nature of solvent-uses etc. Paint Properties – color-tinting strength-reducing power-pigments classification of pigments-pigments properties-oil absorption-refractive index-particle size shape-bleeding-resistance to light and heat.

#### Unit- IV

(18 – Hours)

##### Manufacture of Paints

Ball mill-triple roll mill-bead mill-titrator-high speed and heavy-duty disperser.

##### Important Resins or Modifications of Resins for Paints and Coatings

Epoxy Resins (BPA based resin-curing agents & flame retardant epoxy resins)  
 Alkyds – Introduction of alkyds-different components of it- Modification with rosin-  
 maleic anhydride-acrylics-vinyls-imides etc. Polyester resins-Unsaturated polyester resins-  
 Modification of phenolics such as novolac-epoxy oil soluble and oil reactive Modification  
 of aminor resins (UF & MF) with alcohols and phenols.

**Unit-V**

**(18 – Hours)**

**Synthetic Polymers Chemistry**, Technology of Production-Properties and Applications of  
 Thermoplastic Polymers Polyester:-PET-PBT-Polycarbonate-Poly(amides)-Fluorocarbons  
 (PTFE)-Thermosetting Polymers Silicone-oil-rubber and resin Unsaturated polyesters  
 Polyurethanes

**Text Books:**

- 1.P. Munk & T.M. Aminabhavi, Introduction to Macromolecular Science, 2nd ed. John Wiley & Sons (2002).
- 2.M.P. Stevens, Polymer Chemistry: An Introduction 3rd ed. Oxford University Press (2005).
3. L. H. Sperling, Introduction to Physical Polymer Science, 4th ed. John Wiley & Sons (2005)

**Reference:**

1. Polymer Chemistry - M. P. Stevens, 2nd Ed., Oxford University Press, 1990.
2. Poly. Synthesis - Stanley R. Sandler, Wolf Karo, Vol. 1, Academic Press, Inc., California, 1994.
3. Introduction to Polymer Chemistry - R.B. Seymour, Marcel Dekker, 3rd Ed., (1992)
4. Experiments in Poly. Sci., Collins Bares, F. W. Billmeyer, Wiley Interscience, 1973.
5. Physical Chemistry of Macromolecules. D.D. Deshpande, Vishal Publications, Jalandhar, 1989.
6. Physical Chemistry of Polymers – Hiemenz
7. Organic Polymer Chemistry, V. Jain, IVY Publishing House, New Delhi,
8. Outlines of Paint Technology, W. M Morgan 3rd edn CBS Publishers.
9. Paints, Coatings and solvents, Dieter Stoye, Werner Freitag, Wiley VCH Pub.
10. Encyclopedia of PVC, 2nd Ed., Edited by I Nass, Marcel Dekker Inc., New York.
11. Encyclopedia of Chemical Technology - Kirk and Othemer, Vol.- John Wiley
12. Rubber Chemistry and Technology – Britson

**Question Pattern**

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
IV	20PCH4EC5:2	Polymer chemistry	6	4						
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓		✓	✓	✓		✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO3	✓		✓		✓	✓	✓	✓	✓	✓
CO4	✓		✓		✓	✓	✓	✓		✓
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

<b>Mapping</b>	1-29%	30-59%	60-69%	70-89%	90-100%
<b>Matches</b>	1-14	15-29	30-34	35-44	45-50
<b>Relationship</b>	Very Poor	Poor	Moderate	High	Very High



## SEMESTER – IV

Course Code: 20PCH4EC5:3  
Instruction Hours: 6  
Credits: 4

Exam Hours: 3  
Internal Marks: 25  
External Marks: 75

### ELECTIVE COURSE 5:3 - CHEMISTRY OF NATURAL PRODUCTS

#### Course Outcomes:

- Occurrence, classification and isolation
- Classification, Occurrence And isolation of terpenes
- General nature of anthocyanins, introduction and biological importance of flavones.
- Occurrence and isolation of purines. Classification and spectral properties of steroids.
- Classification- isolation-purification and properties.

#### UNIT-1:

(18 – Hours)

**Alkaloids:** Introduction and functions of alkaloids-General methods of structural elucidation-Structural elucidation-synthesis and biological properties of coniine-piperine-nicotine and papaverine.

#### UNIT-2:

(18 – Hours)

**Terpenoids and Carotenoids:** Terpenoids: Introduction-Isoprene rule-General methods of determining structure-Structure and synthesis of citral-menthol-Geraniol and camphor-Carotenoids: Introduction-geometrical isomerism-Structure determination and synthesis of  $\beta$ -carotene and vitamin-A.

#### UNIT-3:

(18 – Hours)

**Anthocyanines and flavones:** Anthocyanines: Introduction to anthocyanines-Structure and general methods of synthesis of anthocyanines-Cyanidine chloride: structure and determination- Flavones: Structure and determination of flavone and flavonoids-Quercetin: Structure determination and importance.

#### UNIT-4:

(18 – Hours)

**Purines and Steroids:** Purines: Introduction-biological importance-Synthesis and structural elucidation of Uric acid, Xanthine, Caffeine and Theophylline-Steroids: Introduction, stereochemistry and nomenclature- Structural determination and synthesis of cholesterol-Synthesis of ( $\pm$ )-oestrone.

#### UNIT 5:

(18 – Hours)

**Natural Dyes:** Occurrence-colour and constitution-Structural determination and synthesis of indigoitin and alizarin.

**Text books:**

1. O. P. Agarwal, Chemistry of Natural Products, Vol-1, Goel Publishing House, 1997.
2. Gurdeep Chatwal and Anand, Chemistry of Natural Products, Himalayan Publishing Co, 2001

**Reference book:**

1. I. L. Finar, Organic Chemistry, Vol-2, 5th edition, Pearson education, London, 1975.

**Question Pattern**

<b>Section :A (1 Marks)</b>	<b>MCQ Type</b>	<b>20x1=20</b>
<b>Section :B (5 Marks)</b>	<b>Either OR choice</b>	<b>5x5=25</b>
<b>Section :C (10 Marks)</b>	<b>Answer three out of five</b>	<b>3x10=30</b>
<b>Total Marks</b>		<b>75</b>

Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
IV	20PCH4EC5:3	Chemistry of natural products	6	4						
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓		✓	✓	✓		✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO3	✓		✓		✓	✓	✓	✓	✓	✓
CO4	✓		✓		✓	✓	✓	✓		✓
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

Mapping	1-29%	30-59%	60-69%	70-89%	90-100%
Matches	1-14	15-29	30-34	35-44	45-50
Relationship	Very Poor	Poor	Moderate	High	Very High

## SEMESTER – IV

Course Code: 20PCH4CP6  
Instruction Hours: 6  
Credits: 5

Exam Hours: 6  
Internal Marks: 40  
External Marks: 60

### CORE COURSE PRACTICAL 6 - PHYSICAL CHEMISTRY ELECTRICAL PRACTICAL

➤ .  
**Course Outcomes:**

- Practiced the Conductometry titrations.
- Practiced the potentiometric titrations.
- Learn to compare the theoretical values with experimental values.
- Learn the pH measurements.
- Learn the strength of mixture of acids.

**Any ten experiments (to be decided by the course teacher) out of the following experiments.**

1. Conductometry- Acid- alkali titrations.
2. Conductometry- Precipitation titrations.
3. Conductometry- Displacement titrations.
4. Conductometry- Determination of dissociation constant of weak acids.
5. Conductometry- solubility product of sparingly soluble silver salts.
6. Verification of Onsager equation- conductivity method.
7. Determination of degree of hydrolysis and hydrolysis constant of a substance.
8. Potentiometric titrations- Acid alkali titrations.
9. Potentiometric titrations- Precipitation titrations.
10. Potentiometric titrations- Redox titrations.
11. Potentiometry- Determination of dissociation constant of weak acids.
12. Potentiometry- Determination of solubility of silver salts.
13. Potentiometry- Determination of activity and activity coefficient of ions.
14. pH titration of ortho-phosphoric acid.
15. To determine the relative strength of two acids by conductance measurements.
16. To determine the pH of a buffer solution using a quinhydrone electrode.

**References:**

1. J.B.Yadav, "Advanced Practical Physical chemistry", 20th Edn. GOEL publishing House, Krishna Pakashan Media Ltd., (2001).
2. B.P. Levitt, Findlay's "Practical Physical Chemistry" Revised and 9th ed., Longman, London, 1985.
3. J.N. Gurtur and R.Kapoor, "Advanced Experimental chemistry", Vol.I. Chand & Co., Ltd, New Delhi.

### Scheme of valuation

Criteria	Marks
Record	5
Aim and tabulation	10
Calculation	10
Results	
Allowed error 5%	35
5-10%	20
10%<	10

### Relationship Matrix for COs, POs and PSOs

Semester	Code	Title of the Course	Hours	Credits						
IV	20PCH4CP6	Physical chemistry electrical practical	6	5						
Course Outcomes (COs)	Programme Outcomes(POs)					Programme Specific Outcomes(PSOs)				
	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓		✓	✓	✓		✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO3	✓		✓		✓	✓	✓	✓	✓	✓
CO4	✓		✓		✓	✓	✓	✓		✓
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓
Number of Matches(✓) = 42 Relationship: High										

Mapping	1-29%	30-59%	60-69%	70-89%	90-100%
Matches	1-14	15-29	30-34	35-44	45-50
Relationship	Very Poor	Poor	Moderate	High	Very High

## SEMESTER – IV

Course Code: 20PCH4PW

Instruction Hours: 6

Credits: 4

Exam Hours: -

Internal Marks: 20

External Marks: 80

### PROJECT WORK

#### Objectives:

The student can get the knowledge to prepare the document, to implement tools for the specific problem and learn the industrial need programs for their placement.

S.No.	Work Description	Maximum Marks
1	Dissertation	80
2	Viva voce	20
Total		100

#### Note:

#### PASSING MINIMUM – 50 MARKS

##### I Review –December last week

- Confirmation letter from the company
- Project type & title
- Company profile
- Synopsis
- Contact number &mail\_id of the external guide
- S/w selection

##### II Review – January 3<sup>rd</sup> week

- Data or System flow diagram
- Documentation of first three chapters
- Database design
- Input design – Forms
- Output design – Reports

##### III Review – February 3<sup>rd</sup> week

- Complete coding
- Test plan with demo
- Rough documentation of the entire project

##### IV Review – March 1<sup>st</sup> week

- Corrected rough draft
  - Explanation of the entire project
  - Execution of Implementation Work
- Attending all the review is compulsory
- PPT and necessary Documentation should be brought for each Review

- Font size in documentation has to be 12, Times New Roman, Space 1.5
- Document should be neatly aligned and justified
- No change can be made in the review marks later
- Internal mark will be submitted at the same day of review to controller section.

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