

**Curriculum**  
**for**  
**M.Sc Chemistry Programme**  
(For those who were admitted from the academic year 2018-2019 onwards)



Since 1881

**DEPARTMENT OF CHEMISTRY**  
**THE AMERICAN COLLEGE**

An Autonomous Institution Affiliated to Madurai Kamaraj University  
Reaccredited (2<sup>nd</sup> Cycle by NAAC with Grade "A" CGPA-3.46 on a 4-point scale  
**MADURAI-625002**

**THE AMERICAN COLLEGE, MADURAI**  
**PROGRAM / COURSE FRAME ,P.G. DEPARTMENT OF CHEMISTRY (AIDED)**  
**Program for Choice Based Credit System - 2018 – 2019 onwards**

S.N.	Sem	Course Code	Course Title	Hours	Credits	Marks
1	1	PGC 4431	Organic Chemistry – I	6	4	80
2	1	PGC 4433	Inorganic Chemistry – I	5	4	80
3	1	PGC 4435	Physical Chemistry – I	5	4	80
4	1	PGC 4301	Chemistry and Health	4	3	60
5	1	PGC 4303	Organic Qualitative Lab	5	3	60
6	1	PGC 4305	Physical Chemistry Lab – I	5	3	60
<b>Total</b>				<b>30</b>	<b>21</b>	<b>420</b>
7	2	PGC 4432	Organic Chemistry – II	6	4	80
8	2	PGC 4434	Inorganic Chemistry – II	5	4	80
9	2	PGC 4436	Physical Chemistry – II	5	4	80
10	2	PGC 4302	Chemistry in Beauty and Health	4	3	60
11	2	PGC 4304	Organic Quantitative Lab	5	3	60
12	2	PGC 4306	Physical Chemistry Lab – II	5	3	60
<b>Total</b>				<b>30</b>	<b>21</b>	<b>420</b>
13	3	PGC 5531	Organic Chemistry – III	5	5	100
14	3	PGC 5533	Inorganic Chemistry – III	5	5	100
15	3	PGC 5535	Physical Chemistry – III	5	5	100
16	3	PGC 5301	Inorganic Qualitative Lab	5	3	60
17	3	PGC 5601	Research Methodology Lab	10	6	120
<b>Total</b>				<b>30</b>	<b>24</b>	<b>480</b>
18	4	PGC 5532	Organic Chemistry – IV	5	5	100
19	4	PGC 5534	Inorganic Chemistry – IV	5	5	100
20	4	PGC 5536	Physical Chemistry – IV	5	5	100
21	4	PGC 5302	Inorganic Quantitative Lab	5	3	60
22	4	PGC 5602	Project	10	6	120
<b>Total</b>				<b>30</b>	<b>24</b>	<b>480</b>
<b>Grand Total</b>				<b>120</b>	<b>90</b>	<b>1800</b>

## **PG CHEMISTRY –PSO**

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

**PSO-1:** Gain advanced knowledge in major areas of physical, organic, inorganic, analytical environmental and biological chemistry.

**PSO-2:** Isolate, identify and estimate organic/inorganic compounds using classical laboratory and modern analytical methods.

**PSO-3:** Develop skills in literature survey, designing synthetic methodologies and characterizing the ventured compounds.

**PSO-4:** Use ideas, and techniques of chemistry and other fields of science to acquire knowledge in the emerging areas of science.

**PSO-5:** Utilize graphical/virtual communications to interact productively with people from diverse background, employ online search engines and software's tools.

**PSO-6:** Effectively communicate themes relating to chemistry.

**PSO-7:** Develop skills in the handling chemical compounds by identifying their chemical and physical properties including any specific hazards associated with their usage.

**PSO-8:** Actively participate with government agencies in monitoring equity, and supporting nations sustainable development.

**PSO-9:** Pursue research & development in all disciplines of Chemical sciences, succeed in competitive examinations, and emerge as successful entrepreneurs.

**PSO-10:** Develop skills to work with international research and development team, contribute to research collaboration and to be familiar with intellectual property rights both national and globally.

**Mapping of Course Outcomes (COs) with Programme Specific Outcomes (PSOs)**

**–DEPARTMENT OF CHEMISTRY (PG)**

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9	PSO10
PGC 4431	✓			✓		✓	✓		✓	
PGC 4433	✓			✓		✓	✓		✓	✓
PGC 4435	✓			✓		✓	✓		✓	
PGC 4301	✓			✓		✓	✓	✓		
PGC 4303	✓	✓		✓		✓	✓		✓	
PGC 4305	✓	✓	✓	✓			✓		✓	
PGC 4432	✓			✓		✓	✓		✓	
PGC 4434	✓			✓	✓	✓			✓	✓
PGC 4436	✓			✓		✓	✓		✓	
PGC 4302				✓		✓		✓		
PGC 4304	✓	✓		✓		✓	✓		✓	
PGC 4306	✓	✓	✓	✓			✓		✓	

**Mapping of PO and PSO – DEPARTMENT OF CHEMISTRY (PG)**

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
<b>PSO1</b>	✓									
<b>PSO2</b>	✓	✓								
<b>PSO3</b>		✓								
<b>PSO4</b>				✓					✓	
<b>PSO5</b>		✓		✓	✓					
<b>PSO6</b>			✓			✓				
<b>PSO7</b>	✓		✓							
<b>PSO8</b>			✓			✓	✓	✓		
<b>PSO9</b>			✓			✓	✓	✓	✓	
<b>PSO10</b>			✓	✓			✓			✓

**Curriculum**  
**for**  
**First Year M.Sc Chemistry (AIDED) Programme**  
(For those who were admitted from the academic year 2018-2019 onwards)

**SEMESTER I**



Since 1881

**Postgraduate Department of Chemistry**  
**The American College**  
(An Autonomous Institution Affiliated to Madurai Kamaraj University)  
**Madurai, Tamilnadu, INDIA**

**Objectives:**

This is the first of the four semester sequential course in organic chemistry. Students will be dealing with fundamental concepts in organic chemistry, LFER, reactive intermediates, aliphatic, aromatic electrophilic and nucleophilic substitution reactions, UV-Vis and IR spectral techniques.

**Course Outcome:**

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

1. Identify the aromaticity of the molecules and apply basic concepts like inductive and resonance effect to analyze the quantitative relationship between structure and reactivity.
2. Classify the intermediates and identify them in the various rearrangements reactions giving mechanism pertaining to them.
3. Distinguish and analyze mechanisms involved in aliphatic substitution and elimination reactions.
4. Write mechanisms in aromatic nucleophilic and electrophilic substitution reactions and examine the synthetic routes for organic transformations.
5. Calculate the  $\lambda_{\max}$  for the various organic compounds and also able to interpret IR data.

**UNIT-I:**

**Bonding in Organic molecules**

Electrical effects – inductive, electromeric, mesomeric effects and hyperconjugation, tautomerism - Aromaticity in benzenoid and non-benzenoid compounds – Huckel's rule, energy level of  $\pi$  molecular orbitals, annulenes, anti aromaticity, non aromaticity, homo aromaticity.

**Structure and reactivity**

Effect of structure on reactivity – resonance, field and steric effects, Hammond postulates, Curtin-Hammett principle, Quantitative treatment - Hammett equation and linear free energy relationship, substituent and reaction constants - Taft equation.

**UNIT-II:**

**Reactive intermediates**

Carbocations- Synthesis, geometry, memory effect, stability and reactions, rearrangement reactions-Carbanion- Synthesis, geometry, stability and reactions, rearrangement reactions-Free Radical- Synthesis, Structure of radical, radical stability, reactions of radical-Pinacol coupling, McMurry reaction, Acyloin reaction, Selective radical bromination- Carbenes- Synthesis, types of carbenes and their geometry, reactions of carbene- addition to alkene-Simmon-Smith reaction-stereospecific and stereoselective addition to carbenes, insertion reaction, rearrangement reactions-Nitrene.

**Rearrangements reactions**

Migration to electron deficient carbon- Wagner-Meerwein, pinacol-pinacolone, allylic, Wolff-Migration to electron rich carbon-Favorskii, Stevens, Sommet-Hauser, Wittig, Neber- Migration to electron deficient nitrogen-Beckmann, Hofmann, Curtius- Migration to electron deficient oxygen-Baeyer-Villiger, Hydroperoxide, Dakin.

**UNIT-III:**

**Aliphatic nucleophilic Substitution**

The  $S_N2$ ,  $S_N1$ , mixed  $S_N1$  and  $S_N2$ , SET mechanisms-neighbouring group mechanism, participation by  $\pi$  and  $\sigma$  bond, non-classical carbocations- $S_Ni$  mechanism- anchimeric assistance  $S_N1$  mechanism - Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon-reactivity-effect of substrate structure, attacking nucleophile, leaving group, reaction medium-ambident nucleophile and substrate-Phase transfer catalysis of nucleophilic substitution.

**Aliphatic Electrophilic substitution**

Bimolecular mechanism,  $S_E2$  and  $S_{Ei}$ ,  $S_{E1}$  mechanism- Effect of leaving group and solvents.

Elimination reactions

E2, E1 and E1cB mechanism-syn-anti dichotomy-E1-E2-E1cB spectrum-Orientation of the double bond-reactivity- effects of substrate structure, attacking base, leaving group, medium-mechanism and orientation in pyrolytic elimination.

#### UNIT-IV:

##### Aromatic Nucleophilic substitution

The S<sub>N</sub>Ar, S<sub>N</sub>1, benzyne and S<sub>RN</sub>1 mechanism – Reactivity-effect of substrate structure, leaving group, attacking nucleophile.

##### Aromatic Electrophillic substitution

Arenium ion mechanism- orientation & reactivity in mono substituted benzene ring-ortho/para ratio-Partial rate factors-Ipso attack-orientation in other ring systems-Diazonium coupling, Vilsmeier reaction, Gattermann-Koch reaction, Bischler-napieralski reaction-Fries rearrangement.

#### UNIT-V:

##### Addition to Carbon-Carbon multiple bond

Electrophilic, Nucleophilic, Free radical addition-Cyclic mechanism-Addition to conjugated system-Orientation and reactivity.

##### Ultraviolet and visible spectroscopy

Various electronic transitions (185-800nm) – Beer-Lambert's law- effect of solvent on electronic transitions - UV bands for carbonyl compounds, unsaturated compounds, dienes, conjugated polyenes- Feiser- woodward rules for conjugated diene and carbonyl compounds – Fieser-Kuhn rules for polyenes-UV spectra of aromatic and heterocyclic compounds- Steric effect in biphenyls-Applications of UV-visible spectroscopy.

##### Infrared spectroscopy

Molecular vibrations-sample handling techniques- finger print region- Identification of functional groups- interpretations of IR spectra-factors ( hydrogen bonding electronic effects, conjugation, mass effects and ring strain) influencing vibrational frequencies-Applications of IR spectroscopy.

#### References

1. Jerry March, Advanced Organic Chemistry, Reaction mechanism and structure, John Wiley and sons 4<sup>th</sup>Edn., 1992.
2. E.S. Gould, Mechanism and structure in Organic Chemistry, Rinehart & Winston, INC, 1960.
3. Clayden, Greeves, Warren and Wothers, Organic Chemistry, OXFORD University Press, 2007.
4. Peter Skyes, A Guide book to mechanism in Organic Chemistry, Pearson, 2004.
5. C.K. Ingold, Structure and mechanism in Organic Chemistry, Cornell university press.
6. Graham Solomon, Organic Chemistry, John wiley and sons INC 8<sup>th</sup>Edn. 1992.
7. Carey and Sundberg, Advanced Organic Chemistry, Part. A, Structure and mechanism, Planum press 3<sup>rd</sup> Edition, 1990.
8. Willam Kemp, Organic Spectroscopy, Palgrave, 3<sup>rd</sup> edition, 1991.
9. R.M. Silverstein, G.C. Basslerand J.C.Morril, Spectroscopic Identification of Organic compounds, John Wiley & sons INC 5<sup>th</sup> edition 1991.

Mapping of Bloom's Taxonomy with Course Outcome					
	Unit-I	Unit-II	Unit-III	Unit-IV	Unit-V
	CO1	CO2	CO3	CO4	CO5
K1: Remembering	X	X	X	X	X
K2: Understanding	X	X	X	X	X
K3: Applying	X	X	X	X	X
K4: Analyzing	X		X	X	X
K5: Evaluating					
K6: Creating					

**Objective:**

This course deals with the basic concepts like periodic properties, bonding theories and structure. Concepts on acid-base, solid state chemistry, diffraction techniques and nuclear chemistry will also be discussed.

**Course outcome:**

After completion of this course the students will be able to

1. Explain the atomic properties and relate acid base strengths
2. Relate radius ratio rule with structure and ascertain lattice stability & defects
3. Illustrate covalent and metallic bonding and compare the electrical properties in solids
4. Analyze crystal structure and explain solid state reactions
5. Discuss the aspects of nuclear chemistry

**UNIT – I: Basic Concepts**

The modern long form of periodic table – shielding – periodic properties of atoms - ionisation energy and electron affinity – factors affecting – scales of electronegativity – Pauling, Allred-Rochow, Allen scales – acids and bases – Lewis concept – solvent system concept – measure of acid and base strength – steric effect – solvation effect – hard and soft acid base interaction – classification – acid-base strength and hardness, softness – applications of HSAB principle – symbiosis – theoretical basis – Non aqueous solvents – reactions in liquid ammonia, liquid sulphur dioxide – superacids – molten salts

**UNIT – II: Ionic Bonding**

The ionic bond – properties – radius ratio rule – applications – typical crystal structure – AX type – NaCl, CsCl, ZnS, NiAs – AX<sub>2</sub> type – CaF<sub>2</sub>, TiO<sub>2</sub> – lattice energy – Born-Landé equation (no derivation) – Born Haber cycle – implications – limitations of radius ratio rule – covalent character in ionic bond – polarization – layer CdI<sub>2</sub>

Imperfections in solids – classification based on composition – stoichiometric and non stoichiometric – classification based on size and shape – point, line and extended – Fe<sub>3</sub>O<sub>4</sub>, Fe<sub>1-x</sub>O, UO<sub>2+x</sub>

**UNIT – III: Covalent Bonding**

Covalent bonding – VB theory – hybridisation and overlap – VSEPR theory with applications to inorganic compounds and ions – MO theory – MO diagrams for A<sub>2</sub>, AB (Coulson treatment) and AB<sub>2</sub> (BeH<sub>2</sub>, NO<sub>2</sub><sup>-</sup>) molecules – bond energy – bond order

Metallic bond – band theory – electrical properties of solids – conductors, insulators, semiconductors – doping – superconductors – types – Meissner effect – BCS theory – applications

**UNIT – IV: Solid State**

Symmetry – crystal system – Bravais lattice – space groups (H.M notation) – structure factor – scattering factor – x-ray diffraction – single crystal diffraction and powder diffraction – systematic absences – indexing of diffraction data to cubic system – lattice parameter determination – Neutron and electron diffraction – Solid state reactions – types and mechanism

**UNIT – V: Nuclear Chemistry**

Radioactivity – decay constant – half-life period – G.M. counter – scintillation counter – nuclear models – liquid drop model – nuclear fission and nuclear fusion reaction – shell model – nuclear forces, quantization, magic numbers – nuclear accelerators – linear accelerators – cyclotron, synchrocyclotron, betatron – nuclear reactors – fast breeder reactors – applications of radioactivity – solubility determination, neutron activation analysis, radiometric titrations

**References:**

1. Huheey, J. E., Keiter E.A., Keiter R.I., Inorganic Chemistry – Principles of Structure and Reactivity, Harper International, IV Edition, 1993.



2. Shriver D.F. and Atkins P.W., Inorganic Chemistry, Oxford University Press III Edition, 1999.
3. Meissler G.L. and Tarr T.A., Inorganic Chemistry, Pearson Academy, Inc., III Edition, New Delhi, 2004.
4. Porterfield W.W., Inorganic Chemistry, Academy Press, Elsevier, California, 2005.
5. Cotton F.A., Wilkinson G., Advanced Inorganic Chemistry VI Ed., John Wiley and Sons, New York, 1999.
6. William Jolly L., Modern Inorganic Chemistry, Mcgraw-Hill New York, 1985.
7. Greenwood N.N., Ionic Crystals, Lattice Defects and Non-stoichiometry, Butterworths and Co Ltd., 1968.
8. Cotton F.A., Wilkinson G, and Gaus P.L, Basic Inorganic Chemistry, John Wiley and Sons, New York, III Edition 2007.
9. Azaroff. L.V., Introduction to Solids, TataMcGraw Hill Publishing Company, 1995.
10. West A.R., Solid State Chemistry and its Applications, John Wiley and Sons, New York, 1984.
11. Hannay N.B., Solid State Chemistry, Prentice Hall of India Private Limited, New Delhi, 1976.
12. John Wormald, Diffraction Methods, Clarendon Press, Oxford, 1973.
13. Azaroff L.V., Elements of X-ray Crystallography, McGraw Hill, New York, 1968.
14. Jaffe H.H. Milton Orchin, Symmetry in Chemistry, John Wiley and Sons, New York, 1965.
15. Arnikaar H.J., Essentials of Nuclear Chemistry, New Age International (P) Limited, Publishers, New Delhi, IV Edition, 2011.
16. Friedlander G, Kennedy J.W., Edward S. M., Miller J.M., Nuclear and Radiochemistry, John Wiley & Sons. Inc., III Edition, 1981.
17. Glasstone S., Source book on atomic energy, III Edition, Van.DNostrand Company, London 1967.

<b>Mapping of Bloom's Taxonomy with Course Outcome</b>					
	<b>Unit-I</b>	<b>Unit-II</b>	<b>Unit-III</b>	<b>Unit-IV</b>	<b>Unit-V</b>
	<b>CO1</b>	<b>CO2</b>	<b>CO3</b>	<b>CO4</b>	<b>CO5</b>
K1: Remembering	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>
K2: Understanding	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>
K3: Applying	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>
K4: Analyzing		<b>X</b>	<b>X</b>	<b>X</b>	
K5: Evaluating			<b>X</b>		
K6: Creating					

**Course Objectives:**

This is the first course of the five sequential courses in physical chemistry. This course deals with aspects of quantum chemistry, group theory, application of quantum chemistry, group theory approach to bonding and kinetic approach to gases.

**Course outcome:**

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

1. Illustrate the various concepts involved in quantum mechanics and determine the solution for each system.
2. Apply quantum mechanical approach to concepts that govern atomic structure.
3. Assess optical properties, vibrational properties and symmetry operations molecules using group theory.
4. Explain and compare the bonding concepts of chemical systems using quantum and symmetry concepts.
5. Evaluate the distribution, motion and energy of gases.

**UNIT – I: QUANTUM MECHANICS-I**

Black body radiation-photoelectric effect, Need for quantum mechanics-Uncertainty principle-de Broglie equation-The Schrodinger equation (time dependent and time independent) and the postulates of quantum mechanics. Operator algebra – commuting and non-commuting operators – Linear and Hermitian operators – eigen function, eigen values and degeneracy – orthogonality and normalization of wave functions – expansion theorem – eigen value spectrum- Discussion of solutions of the Schrodinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

**UNIT – II: QUANTUM MECHANICS-II**

Approximate methods – The variation theorem – linear variation principle – Perturbation theory (first order and non-degenerate). Application of variation method and perturbation theory to the Helium atom. Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum, operator using ladder operators, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle. Electronic configuration, Russell – Saunders terms and coupling schemes, Slater-Condon parameters, term separation energies of the  $p^n$  configuration, term separation energies for the  $d^n$  configurations, magnetic effects: spin-orbit coupling and zeeman splitting, introduction to the methods of self-consistent field, the virial theorem.

**UNIT – III: GROUP THEORY**

Definition and properties of groups – sub-groups and classes. Symmetry elements and operations – symmetry point groups – identification of the point groups of molecules – representation of groups – matrix representation of symmetry operations – reducible and irreducible representations – construction of character tables – the Great Orthogonality theorem – Molecular vibrations – the symmetry of normal vibrations – determining the symmetry types of the normal modes – contributions of particular internal coordinates to normal modes – selection rules for fundamental vibrational transitions.

**UNIT – IV: BONDING**

QM of bonding – VB & MO theories  $H_2$ ,  $H_2^+$  system – comparison - Huckel theory of conjugated systems, bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene, benzene. Introduction to extended Huckel theory.

Symmetry aspects of MO theory – symmetry factoring of secular equations – carbocyclic systems – LCAO – MO  $\pi$  - bonding. Naphthalene system – symmetry based “selection rules” for cyclization. Hybrid orbitals – hybridization schemes for  $\sigma$  and  $\pi$  bonding – hybrid orbitals as a linear combination of atomic orbitals-selection rules for electronic transition-HCHO, butadiene and benzene system.

**UNIT – V: KINETIC THEORY OF GASES**

Equations of state – molecular speeds – distribution of molecular velocities – one, two and three dimensions(Maxwell distribution of molecular velocity) –Maxwell distribution as energy distribution–Maxwell Boltzmann distribution law – Principle of equipartition energy and quantization – calculation of vibrational heat capacity – transport properties – thermal conductivity in a gas–the molecular collisions and mean free path in a gas – viscosity – diffusion of gases – nonsteady state – Poiseuille formula.

#### References:

1. Walter J. Moore, Physical Chemistry, 5<sup>th</sup> edition, Orient Longman, 1976.
2. Castellan, Physical Chemistry, 3<sup>rd</sup> edition, Addison-Wesley, 1986.
3. Atkins, Physical Chemistry, 7<sup>th</sup> edition, Oxford University Press, 2000.
4. Cotton, Chemical Applications of Group Theory, 3<sup>rd</sup> edition, Wiley, 1998.
5. Chandra, Introductory quantum chemistry, 4<sup>th</sup> edition, TMH, 1994.
6. McQuarrie, Quantum Chemistry, Oxford university press, 1983.
7. Levine, Quantum Chemistry, 5<sup>th</sup> edition, Prentice-Hall, 2003.
8. Hall, Group Theory and Symmetry in Chemistry, 1970.
9. Raman, Group Theory and its application to chemistry, TMH, 1990.
10. Hanna, Quantum mechanics in Chemistry, Benjamin, 1965.

Mapping of Bloom's Taxonomy with Course Outcome					
	Unit-I	Unit-II	Unit-III	Unit-IV	Unit-V
	CO1	CO2	CO3	CO4	CO5
K1: Remembering	X	X	X	X	X
K2: Understanding	X	X	X	X	X
K3: Applying	X	X	X	X	X
K4: Analyzing			X	X	X
K5: Evaluating			X	X	X
K6: Creating					

**Course Objectives:**

This is an introductory course on understanding health in terms of chemistry. This course will attempt to make the students aware of fundamental chemistry of health maintenance with food and medicines, diagnosis of deviation from healthy living, correcting such deviation with medicinal practices and products.

**Course outcome:**

At the end of course, the students should be able to

1. To identify the importance of food in health
2. To correlate the role of various types of chemical constituents in maintenance of health
3. To analyze bio chemical specimens of body by using different diagnostic tools.
4. To apply various medicinal sources and practices in society
5. To ascertain the various routes of administration and application of drugs.

**UNIT –I: Health and food**

Food materials: sources, types – calorific value-Macro and micronutrients – non- dietary foods - balanced diet-imbalance and its consequences- Food and allergy -natural and manmade food materials - food pollution – food contamination-organic food materials- Effect of food materials on body ailments.

**UNIT-II: Health and chemicals**

Health maintenance - Height weight-body mass index-obesity- Healthy skin, hair , bones – Role of enzymes , hormones in health - Nutritional additives-vitamins-micro nutrients -various disorders associated with deficiencies of metal and non metal elements. Sources for various nutrients - fibre content - vitamins etc.

**UNIT- III: Diagnosis and tools**

Traditional methods of diagnosis – Pulse – blood pressure – Analysis of blood, urine, stool, sputum, semen – Normal values of various factors in blood-Reasons for abnormal value of sugar- cholesterol-urea- creatinine - control measures – Microscopy, Endoscopy, Auto-analyser, Differential cell counter, X-ray, ECG,EEG,scanning : ultrasound, echo, CT, MRI,

**UNIT-IV: Drugs and Medicinal practices**

Various sources- animal-plants- earth-microbes - Synthetic drugs –Biotechnology – Human gene therapy – History of drug discovery – serendipity (w.r.t. penicillins, sulpha drugs, clavulanic acid)- Various medical practices: Siddha, Ayurvedha, Unani, Acupuncture, Naturopathy, Allopathy.

**UNIT –V: Drugs and Medicinal preparations**

Requirements of an ideal drug - Need for conversion of drug into medicine – Additives and their role – Various forms of administration of drugs: solid, liquid, semisolid, aerosols, powders, tablet, capsules, suppositories, injectables, syrups, suspensions, ointments, creams – Various routes of administration of drugs: enterals, parenterals, intraadermals etc.,

**References**

1. David Krupadanam.G.L., Vijayaprasad.D, VaraprasadRao.K, Reddy.K.L.N, Sudhakar.C, DrugsUniversitypress(India) Ltd., Orient Longman, First edn.2001.
2. Ramnaiksood, Medical laboratory technology-Methods and interpretation, 3<sup>rd</sup>edn, Jaypee Brothers medical publishers, 1995.
3. Evelyn Pearce, General Text Book of Nursing, ELBS, 1990.
4. JayashreeGhosh, Applied Chemistry, 1<sup>st</sup>Edn, S.Chand& company pvt.Ltd, 2016

Mapping of Bloom's Taxonomy with Course Outcome					
	Unit-I	Unit-II	Unit-III	Unit-IV	Unit-V
	CO1	CO2	CO3	CO4	CO5
K1: Remembering	X	X	X	X	X
K2: Understanding	X	X	X	X	X
K3: Applying	X	X	X	X	
K4: Analyzing			X	X	
K5: Evaluating				X	
K6: Creating					

**Course Objective:**

This lab introduces the qualitative analysis of organic compounds along with separation of organic mixtures.

**Course Outcome:**

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

1. Predict the method for separating the binary organic mixture
2. Apply the basic organic theoretical concepts for analyzing the unknown compound
3. Analyze the elements and functional group present in the individual components
4. Select an appropriate derivative and acquire skills to prepare it
5. Examine the physical properties of the derivative

**Experiments:**

- Separation of organic mixtures
- Elemental analysis
- Functional group(s) identification
- preparation of derivatives
- Physical properties determination (melting point and boiling point)

**References**

1. B. S. Furniss, A.J. Hannaford, P.W.G. Smith, A.R. Tatchell, Vogel's textbook of Practical Organic Chemistry, Pearson, 5<sup>th</sup> edition, 1989.
2. N.S. Gnanpragasam and G. Ramamurthy, Organic Chemistry Lab Manual, S. Viswanathan Pvt. Ltd.

Mapping of Bloom's Taxonomy with Course Outcome					
	CO1	CO2	CO3	CO4	CO5
K1: Remembering	X	X	X	X	X
K2: Understanding	X	X	X	X	X
K3: Applying	X	X	X	X	X
K4: Analyzing			X		X
K5: Evaluating					
K6: Creating					

**Course Objective:**

This lab course incorporates wide range of experiments from various aspects of physical chemistry.

**Course outcome:**

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

1. devise titration using potentiometric and conductometric methods.
2. examine the theories involved in liquid phase adsorption
3. ascertain the order of chemical reaction by kinetic studies
4. assess the phase diagram of systems that forms compound
5. examine the effect of solvent using optical rotation concept

**List of Experiments**

A. PHASE DIAGRAM

1. Two components systems (compound forming)

B. POTENTIOMETRIC METHOD

2. Dissociation constants of weak acid (acetic acid) & pH of buffer solution
3. redox titration (FAS vs  $K_2Cr_2O_7$ )

C. CONDUCTOMETRIC METHOD

4. mixture of strong acid & weak acid vs strong base
5. equivalent conductance of a strong electrolyte & verify the Onsager's equation
6. *Estimation of  $NH_4Cl$*
7. *concentration of mixture of  $HCl$ ,  $HClO_4$  and  $H_2SO_4$*

D. ADSORPTION

8. unknown concentration and the adsorption of oxalic acid from aqueous solutions by activated charcoal & examine the validity of classical and Langmuir's adsorption isotherms

E. KINETICS

9. rate constant and activation energy for ester hydrolysis (at different temperatures for two different concentrations)
10. rate constant and order (potassium persulphate vs potassium iodide)

F. POLARIMETRY

11. *effect of solvent on the optical rotation of camphor*

G. HEAT OF REACTION

12. *effect of solvent on the optical rotation of camphor by polarimetry*

**Demonstration -02; Regular practicals-12; Revision-01; Model Exam-01**

**Reference:**

1. J.B. Yadav, Advanced practical Physical Chemistry, 18<sup>th</sup>Edt, Goel Publishing House, Meerut, 2000
2. B. Viswanathan and P.S. Raghvan, Practical Physical Chemistry, Viva Books Private Ltd., New Delhi, 2009
3. P.C. Kamboj, University Practical Chemistry, Vishal Publishing company, Punjab.2011-2012
4. Saroj Kr Maity and Naba Kr Ghosh, Physical Chemistry Practical, New Central Book Agency Private Ltd., London, 2012

Mapping of Bloom's Taxonomy with Course Outcome					
	CO1	CO2	CO3	CO4	CO5
K1: Remembering	X	X	X	X	X
K2: Understanding	X	X	X	X	X
K3: Applying	X	X	X	X	X
K4: Analyzing	X	X	X	X	X
K5: Evaluating	X			X	
K6: Creating	X				

**Curriculum**  
**for**  
**First Year M.Sc Chemistry (AIDED) Programme**  
**(For those who were admitted from the academic year 2018-2019 onwards)**

**SEMESTER II**



Since 1881

**Postgraduate Department of Chemistry**  
**The American College**  
(An Autonomous Institution Affiliated to Madurai Kamaraj University)  
**Madurai, Tamilnadu, INDIA**

**Course Objectives:**

This is the second of the four semester sequential course in organic chemistry. Students will be dealing with various concepts of Stereochemistry, Conformational Analysis, ORD, CD, Spectroscopy, Natural products and Heterocyclic compounds.

**Course Outcome:**

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

1. Identify the elements of chirality, nomenclature, topicity in the molecules and also apply the various rules to synthesize chiral compounds.
2. Analyze and predict the stability of various conformations and apply ORD, CD curves for identification of absolute configuration of optically active compounds.
3. Identify the spin system present in the molecules, interpret the NMR data and predict the structure of the organic compound using proton and carbon NMR.
4. Apply the 1D-NMR concepts to infer the 2D-NMR data and assess the mass fragmentation pattern followed in various organic compounds.
5. Identify, elucidate the structure of natural products and analyze the basic nature, preparation and reactions of heterocyclic compounds.

**UNIT-I:****Stereochemistry**

Elements of Symmetry-Classification of conformation & configuration based on energy criterion-stereoisomerism, conformations & chirality - racemic modification & classification of racemic modifications, quasi racemates- molecules with more than one chiral center, Nomenclature-D & L, R & S, R\* & S\*, threo and erythro isomers-Pref&Pruf-Prelog system, Brewster system-Stereoisomerism-axial chirality, planar chirality & helicity - allens, spiranes, biphenyls, ansa compounds, cyclophanes, trans-cyclooctene - chirality due to  $sp^3C-sp^3C$  - Topicity&prostereoisomerism-topicity of ligands, groups and faces - homotopic, enantiotopic and diastereotopic atoms, groups and faces – racemization - mechanism of racemization-asymmetric transformation - methods of resolution - optical purity & enantiomeric excess-asymmetric synthesis-substrate controlled-Cram's rule, Prelog's rule-reagent controlled-optically active catalyst-solvent controlled- stereospecific and stereoselective synthesis-Stereochemistry of compounds containing nitrogen, sulfur and phosphorus- pyramidal inversion, 1,3-synaxial interaction, anomeric effect, exo-anomeric effect, Rabbit-ear effect-repulsive gauche effect (hockey sticks effect).

**UNIT-II:****Conformational analysis**

Conformations and stability of mono, disubstituted and trisubstituted cyclohexanes-conformations of cyclohexanone, 2 & 3 alkyl ketone effect-conformations of 2-nalo & 2,6-dihalo cyclohexanones-alkylidenecyclohexanes-conformations of 1,3-dimethylpiperazine, pyranose sugars, 1,3-oxazines, 1,4-oxathiane- conformations and stability mono and disubstituted decalins, perhydrophenanthrenes, perhydroanthracenes-reactivities of cyclohexane, cyclohexanones with respect to oxidation, reduction, substitution and elimination.

**ORD/CD**

Linearly & circularly polarized lights-circular birefringence & circular dichroism-ORD and CD curves: Cotton effect-applications of CD & ORD-use of plane curves-Empirical & semiempirical rules-axial haloketone rule, octant rule.

**UNIT-III:****Proton NMR spectroscopy**

NMR phenomenon- CW and FT NMR- relaxation effects – chemical shifts-factors influencing Chemical shifts ( electro negativity, anisotropic effects and van der Waals' deshielding)- Chemical and magnetic equivalence- exchange phenomenon- spin-spin coupling- Simplification of complex spectra using double resonance techniques, Shift reagents and increased field strength- Classification of spin systems- analysis of AX, AMX, ABX systems- Geminal, vicinal and long range couplings- NOE in stereochemistry.

**Carbon NMR spectroscopy**



#### UNIT-IV:

##### Two dimension NMR spectroscopy

An introduction to 1 – D pulse technique – J-resolved 2-D NMR-2D techniques-HOMCOR, HETCOR, NOESY, DEPT, INEPT, APT and INADEQUATE Techniques.

##### Mass spectrometry

Introduction, ion production – EI, CI, FD, FAB and MALDI-rules of fragmentation-even electron rule, nitrogen rule, Stevenson's rule, rule of thirteen-molecular ion peak, base peak, isotopic peak, metastable peak- McLafferty rearrangement - double hydrogen transfer – prominent fragmentation pattern-mass spectral fragmentation of organic compounds containing common functional groups – hydrocarbons, alcohol, amine, acid, ester, amide, aldehyde, ketone, halocompounds, nitro compound, ether - conjoint spectra.

#### UNIT-V:

##### Natural products

Structural elucidation of Terpenoids ( $\alpha$ -pinene and  $\alpha$ -cadinene)-Alkaloids (quinine and papaverine)-Anthocyanins and flavones (cyanin chloride and quercetin).

##### Heterocyclic Chemistry

Preparation, reactivities, comparison of basicity of heterocyclic compounds with more than one hetero atom–pyrazole - imidazole - isooxazole – thiazole - pyridazine - pyrimidine – pyrazine.

#### References

1. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, New Academic Science, 3<sup>rd</sup> edition, 1991.
2. Ernest L Elliel, Samuel H. Wilen, Stereo Chemistry of Organic compounds, John Wiley & Sons, INC, 2003.
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5. R.M. Silverstein, G.C. Bassler, J.C.Morril, Spectroscopic Identification of Organic compounds, John Wiley & sons INC 5<sup>th</sup> edition 1991.
6. Reg Davis & Martin Frearson, Mass spectrometry, ACOI, John Wiley & Sons, 1989.
7. William Kemp, NMR in chemistry-A multinuclear introduction, Macmillan, 1986.
8. Joseph B. Lambert & Eugene P. Mazzola, Nuclear magnetic resonance spectroscopy, Pearson Prentice Hall.
9. Joseph B. Lambert, Herbert F. Shurvell, Lawrence Verbit, R. Graham Cooks, George H. Stout, Organic structural analysis, Macmillan Publishing CO, Inc, 1976.
10. H. Gunther, NMR spectroscopy: Basic principles, Concepts and Applications in chemistry, 2<sup>nd</sup> edition, Wiley, 1995.
11. I.L. Finar, Organic Chemistry Vol:2, Pearson, 5<sup>th</sup> edition 1975.
12. T. L. Gilchrist, Heterocyclic Chemistry, John Wiley & Sons, Inc., 1985.
13. R.R. Gupta, M. Kumar, V. Gupta, Heterocyclic Chemistry, Vol-I & II, Springer, 1998.
12. J.A. Joule and K. Mills, Heterocyclic Chemistry, Wiley, 5<sup>th</sup> edition, 2010.
13. R.M. Acheson, An introduction to the chemistry of heterocyclic compounds, John Wiley, 3<sup>rd</sup> Edition, 2008.

Mapping of Bloom's Taxonomy with Course Outcome					
	Unit-I	Unit-II	Unit-III	Unit-IV	Unit-V
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K2: Understanding	X	X	X	X	X
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K4: Analyzing		X	X	X	X
K5: Evaluating				X	
K6: Creating					

**Course Objective:**

The coordination chemistry of transition metal complexes, spectral tools normally employed for characterization, reactivities of complexes with reaction mechanisms will be discussed in this course.

**Course outcome:**

After completion of this course the students will be able to

1. Differentiate transition series, relate coordination number with geometry and explain complex stability & isomerism
2. Describe and examine the bonding in coordination compounds
3. Infer the magnetic properties, electronic and NQR spectral data
4. Interpret and deduce the structure of complexes using IR, NMR, MB and EPR spectra
5. Differentiate the synthetic pathways, reaction mechanism and relate their rates

**UNIT – I: General concepts in coordination chemistry**

General view of transition metals and coordination chemistry - size, variable oxidation state, catalytic property - comparison of first, second and third transition series – nomenclature – Structure and coordination number – higher coordination numbers – isomerism – types - stability of complexes – complex equilibria – factors affecting stability - chelate effect - determination of stability constants – Job's method - ORD and CD - ligand conformation

**UNIT – II: Theories of coordination compounds**

Theories of bonding – VBT – principles — defects – CFT – CFSE – Octahedral symmetry – Tetrahedral symmetry – factors affecting CFSE – Applications of CFSE – Jahn-Teller distortion – consequences – Square planar complexes – limitations of CFT – evidences of metal-ligand covalency – LFT – MOT of octahedral and tetrahedral complexes – sigma & pi bonding in MOT

**UNIT – III: Magnetic properties, electronic and NQR spectra**

Electronic Spectroscopy – Term Symbols – Orgel diagrams – intensities, Shapes of peaks - assignment of transitions - calculation of crystal field parameters for  $d^3$ ,  $d^8$  systems – charge transfer spectra – types

Magnetic property of complex ions – types of magnetic property – groups with small and large multiplet separation – orbital contribution to magnetic moment

NQR – principle – eQq – interpretation – effect of crystal lattice – structural information

**UNIT – IV: IR, NMR, MB and EPR spectra**

Vibrational spectroscopy – applications - symmetry and coordination site – complexes of aqua, cyano, nitro, nitrito, urea, acetylacetonato ligands

NMR – applications –  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$ ,  $^{17}\text{O}$ ,  $^{31}\text{P}$ ,  $^{19}\text{F}$  – paramagnetic complexes – contact shift, pseudo contact

Mossbauer spectra – principle – isomer shift – electron environment – quadrupole interaction – application

EPR – g value – presentation of spectrum – hyperfine splitting – factors affecting g value – application to Cu(II) complexes – zero field splitting and Kramer's degeneracy, metal ligand covalency

**UNIT – V: Reactions of metal complexes**

Reaction mechanisms of transition metal complexes- classification – anation – aquation and base hydrolysis – acid hydrolysis – stereo chemistry of the products – factors affecting the rate – nucleophilic substitution reactions of square planar complexes - Trans effect - theories – polarization,  $\pi$ -bonding – electrons transfer reactions – inner and outer sphere reaction – mechanism - template effect

**References:**

1. Huheey J.E, Keiter E.A, Keiter R.L, Medhi O.K, Inorganic Chemistry - Principles of structure and Reactivity, Pearson Education, ISBN 81-7758-130-9, 2006.
2. Cotton F.A and Wilkinson, G., Advanced Inorganic Chemistry, John Wiley and Sons, New York VI Edition 1999.
3. Purcell K.F and Kotz J.C., Inorganic Chemistry, Saunders, Philadelphia, 1977.

4. Meissler G.L. and Tarr T.A., Inorganic Chemistry, Pearson Academy, Inc., III Edition, New Delhi, 2004.
5. Shriver D. F and Atkins P.W, Inorganic Chemistry, oxford univ. Press 1999
6. Ebsworth E.A.V, Rankin D.W.H, Cradock S, Structural Methods in Inorganic Chemistry, Wiley-Blackwell illustrated edition, 1986.
7. Kettle S.F.A, Coordination Compounds, The ELBS and Nelson, 1969.
8. Drago, R.S Physical Methods in Inorganic Chemistry, Reinhold, NY 1965.
9. Drago, R.S Physical Methods in Chemistry, W.B. Saunders Philadelphia 1977.
10. Lever, A.B.P., Inorganic Electronic Spectroscopy, Elsevier., Amsterdam II Edition.
11. Figgis, B.N., Introduction to ligand fields, Interscience, NY 1996.
12. Sutton D., Electronic spectra of transition metal complexes, McGraw-Hill, London, 1968.
13. Nakamoto, Kazuo, Infrared and Raman Spectra of Inorganic and Coordination Compounds, IV edition, John Wiley and Sons, NY, 1986.
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<b>Mapping of Bloom's Taxonomy with Course Outcome</b>					
	<b>Unit-I</b>	<b>Unit-II</b>	<b>Unit-III</b>	<b>Unit-IV</b>	<b>Unit-V</b>
	<b>CO1</b>	<b>CO2</b>	<b>CO3</b>	<b>CO4</b>	<b>CO5</b>
K1: Remembering	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>
K2: Understanding	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>
K3: Applying	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>
K4: Analyzing	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>
K5: Evaluating				<b>X</b>	
K6: Creating					

**Course Objectives:**

This is the second course in the four sequential courses in physical chemistry. This course deals with rotational, vibrational, electronic, nuclear magnetic resonance spectroscopy, EPR, NQR and Mossbauer Spectroscopy.

**Course outcome:**

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

1. Ascertain the spectral lines of molecules that are active in rotational and vibrational spectroscopy
2. Apply Raman and electronic Spectroscopy concepts for different molecules.
3. Examine NMR active systems on the basis of quantum mechanics
4. Apply vector diagram and pulse sequence for various  $^1\text{H}$  and  $^{13}\text{C}$  NMR techniques.
5. Illustrate the principle involved in ESR, NQR and Mossbauer Spectroscopy and distinguish chemical species using these spectroscopy.

**UNIT – I: ROTATIONAL AND VIBRATIONAL SPECTROSCOPY**

Rotation spectroscopy – rotation of molecules and rotational spectra rigid diatomic molecule – intensities of spectral lines – effect of isotopic substitution – non-rigid rotator – spectrum of non-rigid rotator – linear polyatomic molecules – symmetric top molecule – asymmetric top molecule

Introduction to vibration – rotation spectroscopy – energy of diatomic molecules – simple Harmonic Oscillator – Anharmonic Oscillator – Diatomic vibrating rotator – breakdown of Born-Oppenheimer approximation – normal modes and normal coordinates – overtone and combination bands – influence of rotation on the spectra of polyatomic linear molecules with parallel and perpendicular vibrations – symmetric top molecules with parallel and perpendicular vibrations – effect of nuclear spin – FT-IR.

**UNIT – II: RAMAN AND ELECTRONIC SPECTROSCOPY**

The Raman effect – quantum mechanical and classical approach to Raman effect – polarizability – Pure rotational Raman spectra of linear, symmetric top, spherical top and asymmetric top molecules – vibrational Raman spectra – Rule of mutual exclusion – IR and Raman active frequencies – Fermi Resonance – rotational fine structure – depolarization ratio – vibrations of spherical top molecules – The Laser source – production and energy level studies of gas, solid and liquid state lasers – Applications of laser Raman Spectroscopy – Structural determination – polarized and depolarized Raman lines – Resonance Raman Spectroscopy – surface-enhanced Raman scattering– Non-linear Raman effects – Hyper Raman effect– Stimulated Raman effect – Inverse Raman effect –Coherent anti-stoke Raman (CARS) Spectroscopy – Time resolved Raman Spectroscopy.

Electronic spectra of molecules – Born-Oppenheimer approximation – vibrational coarse structure – Frank-Condon principle – rotational fine structure of electronic – vibration transitions – Fortrat diagram – pre-dissociation.

Basic principles – photo-electric effect – ionization process – Koopman's theorem – photoelectron spectra of simple molecules – ESCA – chemical information from ESCA – Auger electron spectroscopy – basic idea.

**UNIT – III: NMR-I**

Nuclear spins and magnetic moments – resonance condition – Larmor precession– relaxation – population of energy levels –Bloch equation – NMR spectrum – chemical shift – factors affecting chemical shift values – spin-spin coupling – quantum mechanical formulation – Hamiltonian operator for high resolution NMR  $A_2$  system, AB system and AX system – direct analysis AB system,  $AB_2$  system and ABX system.

Double resonance experiments – spin decoupling – spin tickling – NOE – INDOR – hetero nuclear double resonance broadband and off-resonance decoupling – CIDNP – Dynamic NMR.

**UNIT – IV: NMR-II**

<sup>1</sup>H NMR: FT-NMR instrumentation – pulse FT NMR – relaxation mechanisms – relaxation time determination of T1 and T2–gated decoupling

<sup>13</sup>C NMR:1D NMR – SEFT, SPI, INEPT, DEPT and INADEQHATE – 2D NMR experiments – presentation of 2D NMR spectrum – COSY – HOMCOR, HETCOR, HMQC, HMBC, NOESY – 2D INADEQUATE – J-resolved spectra

Chemical shift and charge density calculation – computation of <sup>13</sup>C chemical shift values using tables – theory of geminal coupling, vicinal coupling and long-range coupling – Solid state NMR.

## UNIT – V: ESR, NQR AND MOSSBAUER SPECTROSCOPY

**EPR:**esr. experiment – thermal equilibrium and relaxation – experimental methods and instrumentation – magnetic field modulation – g-factor – absorption intensity and concentration measurements – factors influencing the absorption line-shape – hyperfine structure and its energy levels – interpretation of e.s.r spectra in solution – anisotropic systems – triplet state – energy levels for Kramer’s doublets

**NQR:** introduction – general principles – experimental detection of N.Q.R frequencies – chemical bonding – substituent effects – interpretation of <sup>14</sup>N quadrupole coupling constants

**Mossbauer spectra:**basics – recoilless emission and absorption – spectrum – experimental methods – hyperfine interactions

### References:

1. W. J. Moore, Physical Chemistry, 5<sup>th</sup> edition, Orient Longman, 1976.
2. Atkins, Physical Chemistry, 7<sup>th</sup> edition, Oxford University Press, 2000.
3. C.N. Banwell, Fundamentals of Molecular Spectroscopy, 4<sup>th</sup> edition, TMH, 1997.
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14. D. N. Sathyanarayana, Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR, 2 – e, I K International Publishing House, 2013.

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K4: Analyzing	X		X		X
K5: Evaluating					
K6: Creating					

**Course objectives:**

This course is intended to impart awareness about healthy human living maintaining a beautiful appearance. There will be a study on hygienic practices, maintaining skin, hair and physique to enhance natural beauty.

**Course outcome:**

**At the end of course, the students should be able**

1. To diagnose the problems and solutions for hygienic living
2. To apply the hair care products for maintaining and beautifying the hair.
3. To discuss the functions, problems of skin and make it have a good appeal
4. To formulate beauty enhancers connected with colours and pigments.
5. To determine the good physique fitness.

**Unit I: Hygiene and Appearance**

Hygiene and civilisation-bathing and clothing-soap and bath oils and essences -cleansing and cold creams-antiperspirants and deodorants-

Functions of dentifrices-characteristics, ingredients and formulation of tooth pastes/toothpowders- composition and formulation of mouthwashes-naturopathic medical practices-factors affect skin-skin care in different seasons-silver nanoparticles in cosmetics-sources and extraction of perfumes from natural sources.

**Unit II: Hair and Beauty**

Hair-structure, types and functions-ailments of hair-steps to keep hair healthy-hair care products-composition, characteristics and formulation of shampoos/anti-dandruff shampoos-characteristics, classification and formulation of hair colourants.

Hair waving- chemistry of temporary and permanent hair waving-conditioners-neutralizer-methods of hair straighteners-unwanted hairs-depilation and epilation-shaving preparations before and after shaving.

**Unit III: Skin and Beauty**

Structure and functions of skin- skin colour- nutrients for skin-problems of the young skin and aging of the skin- raw materials and its characteristics, formulation of skin care products-moisturising creams, nourishing cream and emollient cream- herbal extracts and essential oils in skin care-

Sunshine and suntan-sun protection factor-skin bleaches

Skin creams- cleansing and cold creams-characteristics-types of cleansing creams-general procedure for manufacturing-vanishing cream and its procedure of formulation-sunscreen preparations-principle and formulae.

**Unit IV: Beauty Enhancers**

Social trends in use of makeup products- colour and pigments in cosmetics-face powder and talcum powder-vanishing and foundation creams-rouges and blushers-eye makeups: mascara, eyeshade, eyeliner, eyebrow and kohl

Lipstick-characteristics of lipstick- basic raw materials and its role in formulation of lipstick-tests for lipsticks

**Unit V: Physique and Beauty**

Symmetry in human body-height, weight and body mass index-daily habits and health-chemistry of maintaining body structure and appearance-physical exercise- yoga, walking, jogging and gym- wrong postures and effects-food habits and diets-clothing and beauty.

**References:**

1. B. M. Mithal & R. N. Saha, A handbook of cosmetics, VallabhPrakashan Publication, New Delhi, 2000
2. Science and the beauty business, John V. Simmons. V.1, The science of cosmetics. Macmillan Education,

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K4: Analyzing			X	X	
K5: Evaluating				X	
K6: Creating					

**Course Objectives:**

This lab introduces the quantitative analysis and preparation of organic compounds. Various purification techniques will be carried out.

**Course Outcome:**

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

1. Estimate the quantity of organic compounds
2. Apply the basic organic theoretical concepts for designing a scheme for synthesis of organic compounds
3. Identify the methodology to purify the compounds
4. Examine the formation of products with chromatography techniques
5. Develop expertise for future research

**Experiments**

**Volumetric analysis**

1. Estimation of phenol/aniline
2. Estimation of glucose (Bertrand's method)
3. Estimation of glucose (Lane and Eynon method)
4. Estimation of ketone
5. Estimation of formaldehyde/carbonyl compounds

**Preparation (Two-stage)**

1. Nitroacetanilide → p-bromoacetanilide → p-bromoaniline
2. Benzophenone → benzophenoneoxime → benanilide
3. Benzoin → benzil → benzilic acid
4. 4-nitrotoluene → 4-nitrobenzoic acid → 4-aminobenzoic acid

**Analytical methods**

1. Chromatography
  - a. TLC – separation of organic mixtures
  - b. column chromatography – purification of organic mixtures
2. Reduced pressure distillation
3. Extraction of caffeine
4. Extration of pigments/terpenoids-Soxhlet method
5. Recrystallization techniques

**References**

1. B. S. Furniss, A.J. Hannaford, P.W.G. Smith, A.R. Tatchell, Vogel's textbook of Practical Organic Chemistry, Pearson, 5<sup>th</sup> edition, 1989.
2. N.S. Gnanpragasam and G. Ramamurthy, Organic Chemistry Lab Manual, S. Viswanathan Pvt. Ltd.
3. N.K. Vishnoi, Advanced Practical Organic Chemistry, Vikas Publishing, 1<sup>st</sup> edition, 1979.

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K5: Evaluating		X			X
K6: Creating		X			X



**Course Objectives:**

This lab course covers the various physical chemistry concepts there by enhance subject understanding.

**Course outcome:**

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

1. Explain distribution of solute in the mixture of immiscible solvents
2. Examine viscosity of mixture of liquids
3. Apply spectrophotometry for binary coloured liquids
4. Deduce the various constants involved in ionic equilibrium
5. Assess three component phase diagram

**List of Experiments**

A. PHASE DIAGRAM

1. three component system: acetic acid, chloroform and water

B. POTENTIOMETRIC METHOD

2. Mixture of KCl and KI vs  $\text{AgNO}_3$  & calculate their solubility product
3. mixture of strong acid & weak acid vs strong base & calculate their dissociation constant

C. CONDUCTOMETRIC METHOD

4. hydrolysis constant of freshly prepared and dried aniline hydrochloride
5. *mixture containing oxalic acid and acetic acid using alkali*
6. solubility product of barium sulphate (barium chloride vs potassium sulphate)
7. mixture of  $\text{H}_2\text{SO}_4$ ,  $\text{CH}_3\text{COOH}$  and  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$  vs alkali

D. SPECTROPHOTOMETRY

8. *binary mixture composition (potassium dichromate and potassium permanganate)*

E. VISCOSITY

9. Viscosity, composition & validity of J. Kendall's equation of different mixtures (nitrobenzene and Benzene (or) toluene and  $\text{CCl}_4$ )

F. DISTRIBUTION METHOD

10. distribution co-efficient (benzoic acid in benzene/water & prove its dimerisation in benzene)
11. *formula of complex ion (formed between cupric ion and ammonia)*
12. *distribution co-efficient ( $\text{I}_2$  in  $\text{CCl}_4$  / water)*

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4. Saroj Kr Maity and Naba Kr Ghosh, Physical Chemistry Practical, New Central Book Agency Private Ltd., London, 2012

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K6: Creating					
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**Curriculum**  
**for**  
**Second Year M.Sc Chemistry (AIDED) Programme**  
(For those who were admitted from the academic year 2018-2019 onwards)

**SEMESTER III**



Since 1881

**Postgraduate Department of Chemistry**  
**The American College**  
(An Autonomous Institution Affiliated to Madurai Kamaraj University)  
**Madurai, Tamilnadu, INDIA**

**Course Objectives:**

This is the third of the four semester sequential course in organic chemistry. This course deals with oxidation and reduction reactions, photochemical and pericyclic reactions in addition to organometallic reagents.

**Course Outcome:**

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

1. Analyze the various oxidizing reagents to effect organic transformations.
2. Use the various reducing reagents and synthesize organic compounds.
3. Predict the product along with stereochemical nature of the reactions under photochemical conditions.
4. Compare various rules in pericyclic reactions to predict product and their stereochemistry.
5. Identify the potential use of various organometallic reagents and apply them to synthesize compounds

**UNIT-I : Oxidation Reactions**

DMSO -Swern oxidation,  $\text{HIO}_4$ ,  $\text{Pb}(\text{OAc})_4$ ,  $\text{Hg}(\text{OAc})_2$ ,  $\text{I}_2 / \text{AgOAc}$  (dry and wet)- Woodward and Prevost, Peroxides- Sharpless asymmetric epoxidation and dihydroxylation, Peroxyacids, PCC (Corey's reagent), PDC, Etards reagent, Jones reagent,  $\text{MnO}_2$ ,  $\text{OsO}_4$ , DDQ,  $\text{SeO}_2$ ,  $\text{N}_2\text{O}_4$  and Wacker reagent ( $\text{PdCl}_2$ ), Oxidation with Ruthenium tetroxide, Iodobenzene diacetate, Thallium (III) nitrate.

**UNIT-II : Reduction Reactions**

Complex metal hydrides such as  $\text{LiAlH}_4$ ,  $\text{NaBH}_4$ ,  $\text{Na}(\text{CN})\text{BH}_3$ ,  $\text{Zn}(\text{BH}_4)_2$  and trialkyl tin hydrides-Dissolving metals such as alkali metals, tin and zinc- $\text{H}_2$ /various metal catalysts (hydrogenation)- $\text{SnCl}_2$ , Lawesson's reagent –  $\text{TiCl}_4 / \text{Zn-Cu}$  (Mac Murra's reagent) –  $\text{TiCl}_4 / \text{Mg-Hg}$ -Wilkinson's catalyst, Lindlar catalyst- $\text{BH}_3/\text{THF}$ , 9-BBN, optically active boranes-Baker's yeast

**UNIT-III : Photochemistry**

Introduction - Jablonski diagram - geometry of excited states - quenching - sensitisation - quantum efficiency - introduction to photo chemical reaction - photo sensitized reaction - reactivity of electronically excited ketones - Norrish-I and Norrish-II reactions - photo reductions - Paterno Buchi reaction – Barton's reaction – photo addition – photo oxidations (di- $\pi$  methane or Zimmerman rearrangement) - photo Fries rearrangement - photo chemistry of  $\alpha$ ,  $\beta$  unsaturated compounds – photo chemistry of arenes – photo chemistry of vision.

**UNIT-IV : Pericyclic reactions**

Atomic and molecular orbitals - Electro cyclic reaction - concepts of con and dis rotation - stereochemical course of electro cyclic reaction in terms of conservation of orbital symmetry - cyclization of butadienes and 1,3,5- hexatriene - Frontier-Molecular orbital approach - orbital correlation diagram - state correlation diagram - theory of cyclo additions [4+2] and [2+2] additions - suprafacial and antarafacial additions - Diels alder reactions - endoselectivity regioselectivity - catalysis of Lewis acid theory of sigma tropic reactions - sigma tropic migrations of hydrogens and carbons - Claisen, Cope and Aza-Cope rearrangements - Fluxional tautomerism.

**UNIT-V : Organometallic reagents**

Organometallic reagents- principle, preparation, properties and applications of the following in organic synthesis with mechanistic details Cu, Li (Shapiro reaction), Mg, Pd, B, Rh, Si, Ti, Hg, Cd, Zn, P, Cr.

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Mapping of Bloom's Taxonomy with Course Outcome					
	CO1	CO2	CO3	CO4	CO5
K1: Remembering	X	X	X	X	X
K2: Understanding	X	X	X	X	X
K3: Applying	X	X	X	X	X
K4: Analyzing	X	X		X	
K5: Evaluating		X		X	
K6: Creating		X			

**Course Objective:**

This course exposes students to a detailed discussion on organometallics, some aspects of bioinorganic and f-block elements.

**Course Outcome:**

After completion of the course the students will be able to:

1. Describe the bonding and deduce the structure & stability of sigma and pi complexes
2. Illustrate the catalytic property of organo-metallic compound
3. Explain and highlight the properties of f-block elements
4. Discuss the structure and functions of metalloenzymes
5. Reason the role of metals in redox proteins, diagnosis and medicine

**UNIT – I: ORGANOMETALLIC CHEMISTRY - I**

Stability of organometallic compounds – effective atomic number rule – theoretical basis – metal carbonyls – preparation, properties and structures – carbonylate anions – carbonyl hydrides – synthetic utility – metal nitrosyls - preparation-bonding - stereochemical control of valence – dihydrogen complexes – carbocyclic systems – benzene, cp, cht, cot, cyclobutadiene – synthesis of ferrocene – reactions – MO diagram – alkene, alkyne, carbene and carbyne metal complexes – synthesis, structure and bonding – fluxional behavior

**UNIT – II: ORGANOMETALLIC CHEMISTRY- II**

Coordinative unsaturation – oxidative addition – reductive elimination – agostic interaction – activation of small molecules – insertion and elimination – nucleophilic attack on coordinated ligands – catalysis by organometallic compounds – hydrogenation cycle – hydroformylation – Monsanto acetic acid process – Wacker process – isomerisation reaction – WGS reaction - synthesis of gasoline – Fischer Tropsch process – Mobil process – olefin metathesis- Zeigler – Natta catalysis.

**UNIT – III: THE f-BLOCK ELEMENTS**

General features – occurrence –variable valencies - lanthanide and actinide contraction – separation of lanthanides – absorption spectra of Ln – magnetic properties– coordination chemistry – applications - shift reagents – transactinide elements – chemistry of uranium –uranyl complexes – extraction cycles of U and Np.

**UNIT – IV: BIOINORGANIC CHEMISTRY- I**

Essential and trace elements in biological systems – biological significance of metals – alkali & alkaline earth metals – Na/K pump – transition metal storage and transport of Fe, Cu, Zn – biological oxygen transport systems - structure and function of heme and non- heme proteins (Mb, Hb, Hc, Hr) – non-redox metalloenzymes - carboxy peptidase - carbonic anhydrase.

**UNIT –V: BIOINORGANIC CHEMISTRY- II**

Metalloproteins in electron transport processes – Functions of Fe, Cu proteins- cytochrome C – cytochrome P-450 – iron - sulphur proteins – blue copper proteins- superoxide dismutase – nitrogen fixation – coenzyme B<sub>12</sub>- metal-nucleic acid interactions- fundamental reactions of metals with nucleic acids – metals in diagnosis and medicine –chelate therapy.

**References:**

1. Huheey J.E., Inorganic Chemistry IV Edn. Principles of Structure and Reactivity, Collins College Publishers, New York 1993.
2. Cotton, F.A. and Wilkinson, G.I., Advanced Inorganic Chemistry VI Edn. John Wiley and Sons, New York, 2004.
3. Purcell, K.F. and Kotz, J.C., Inorganic Chemistry, Saunders, Philadelphia, 1977.
4. Powell, P., Principles of Organometallic Chemistry II Edn. Chapman and Hall, New York, 1988.
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9. Bertini I Gray and others, Bioinorganic Chemistry – Viva Books Pvt. Ltd., 1998.
10. Lippard S.T. Berg T.M., Principles of Bioinorganic Chemistry, Panima publishing Co. New York 1997.
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<b>Mapping of Bloom's Taxonomy with Course Outcome</b>					
	<b>Unit 1</b>	<b>Unit 2</b>	<b>Unit 3</b>	<b>Unit 4</b>	<b>Unit 5</b>
	<b>CO1</b>	<b>CO2</b>	<b>CO3</b>	<b>CO4</b>	<b>CO5</b>
K1: Remembering	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>
K2: Understanding	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>
K3: Applying	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>
K4: Analyzing	<b>X</b>		<b>X</b>		<b>X</b>
K5: Evaluating	<b>X</b>				
K6: Creating					

**Course objectives:** The learners should be able to apply chemical thermodynamic concepts in understanding the physical behaviour of solution mixtures, utilize elementary laws of chemical kinetics in chemical reactions, acquire analytical skills in the field of photochemistry & radiation, apply theories of electrochemistry to understand electrode kinetics and theoretical aspects of electrochemical application.

**Course outcome:**

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

1. Relate the effect of solute on thermodynamic properties of solution.
2. Deduce the rate of chemical reactions to understand mechanism involved in reactions.
3. Examine the changes on molecules using radiation.
4. Determine thermodynamic properties of electrochemical cells.
5. Explain redox process at the electrode and determine the kinetics of such process.

**UNIT – I: CHEMICAL THERMODYNAMICS**

A general review of enthalpy, entropy and free energy concepts, Genesis of third law and its limitations – Thermodynamics of systems of variable compositions – partial molar quantities and their determination – chemical potential – Gibbs-Duhem equation – Duhem-Margules equation – Fugacity and its determinations – choice of state- Activity and activity coefficients – electrolytes and non-electrolytes – equilibrium thermodynamics - Gibbs phase rule and its application to three component systems – Introduction to non-equilibrium thermodynamics – transformations of the generalized fluxes and forces, non-equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations.

**UNIT – II: CHEMICAL KINETICS – I**

Simple collision theory, absolute reaction rate theory, thermodynamics treatment, potential energy surfaces, application of ARRT to simple bimolecular processes – steady state approximation, principle of microscopic reversibility & detailed balancing – chain reactions – general characteristics, study of kinetics of chain reactions like – decomposition of acetaldehyde and  $\text{N}_2\text{O}_4$ ; study of  $\text{H}_2\text{-O}_2$  explosive reactions. Theory of unimolecular reactions – Lindemann, Hinshelwood, RRKM and Slater treatments. Reactions in solutions – factors influencing reaction rate in solution, significance of dielectric constant, salt effect, and kinetic isotope effect. Oscillatory reactions.

**UNIT – III: PHOTOCHEMISTRY AND RADIATION CHEMISTRY**

Physical properties of the electronically excited molecules – excited state dipole moments excited state  $\text{pK}_a$ , excited state redox potential. Fluorescence, phosphorescence and other deactivation process – Stern-Volmer equation and its applications. Photosensitisation and chemiluminescence. Experimental techniques in photochemistry – flash photolysis technique.

Radiation chemistry – source of high energy – interaction of high energy radiation with matter, radiolysis of water – definition of G value. Primary and secondary process, linear energy transfer – the hydrated electron and its reactions.

**UNIT – IV: ELECTROCHEMISTRY – I**

The nature of electrolytes –ion-ion and ion-solvent interactions. Mean ion activity-The Debye-Huckel equation – Bjerrum equation- Conductivity - transport numbers – Nernst Einstein equation - Stork Einstein equation- Debye-Huckel Onsager equation - Conductivity at high frequency and at high field strength. Determination of transport number.



Double layer-polarized and non-polarized electrodes – Lippmann equation – Models for double layer – Helmholtz, Guoy&Chapmann – Stern models – Zeta potential – Electro-kinetic phenomena – Electro-osmosis. Streaming potential – electrophoresis.

## UNIT – V: ELECTROCHEMISTRY – II

Electrode potential – Types of potential generation – Nernst equation – Hydrogen scale – other reference electrodes – concentration cells – Liquid junction potential – membrane equilibria. Butler-Volmer equation – Tafel equation – electrolysis & overvoltage – Theories of hydrogen overvoltage – Application of EMF measurements & conductivity. Batteries – fuel cells – corrosion. Zero current potentiometry - constant current potentiometry. Polarography – pulse polarography – Differential pulse polarography – stripping voltammetry. Cyclic voltammetry – electrogravimetry – colorimetric methods

## REFERENCES

1. Klotz and R.M. Rosenberg, Chemical Thermodynamics, 4<sup>th</sup> edition, Benjamin, 1986.
2. Kuriacose and Rajaram, Thermodynamics, 3<sup>rd</sup> edition, S.N. Chand, 1999.
3. W.J. Morre, Physical Chemistry 5<sup>th</sup> edition, Orient Longman, 1976.
4. Castellan, Physical Chemistry, 3<sup>rd</sup> edition, Addison Wesley, 1983.
5. Lee, Sears and Turcotte, Statistical Thermodynamics, 2<sup>nd</sup> edition, Addison Wesley, 1973.
6. Glasstone, Introduction to Electrochemistry, Von Nostrand
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8. Rock, Chemical Thermodynamics, Oxford University press, 1983.
9. Crow, Principles and applications of electrochemistry, Chapman and Hall, 1988.
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13. Spinks, T.W.T., An introduction to Radiation Chemistry, John Wiley & sons, 1964.

Mapping of Bloom's Taxonomy with Course Outcome					
	Unit-I	Unit-II	Unit-III	Unit-IV	Unit-V
	CO1	CO2	CO3	CO4	CO5
K1: Remembering	X	X	X	X	X
K2: Understanding	X	X	X	X	X
K3: Applying	X	X	X	X	X
K4: Analyzing		X	X	X	X
K5: Evaluating		X			
K6: Creating					

**Course Objective:**

This is a laboratory course that deals with the principles and methods of qualitative analysis of common and less common cations present in a mixture.

**Course Outcome:**

After completion of the course the students will be able to:

1. Summarise the principle of distribution of common and less common cations in different groups
2. Demonstrate reactions for identification of cations
3. Develop analytical skill in the field of separation of cations from mixture.
4. List the cations present in a mixture
5. Design methods to analyze industrial effluents, antique pieces, environmental samples etc.,

**Component 1: Theoretical principles**

1. Classification of cations into analytical groups and classification within each analytical group.
2. Confirmatory and spot test for cations – Chemistry of reactions

**Component 2:**

1. Semimicro qualitative analysis mixtures of four simple salts containing two common cations and two less common cations with non-interfering anions.

Common cations of:

- Group I: Pb and Hg;
- Group II: Hg, Cu, Cd, Bi, Sb, As, and Sn;
- Group III: Al, Fe, and Cr;
- Group IV: Mn, Zn, Co, and Ni
- Group V: Ca, Sr, and Ba
- Group VI: Mg, K, and  $\text{NH}_4^+$

Less common cations of:

- Group I: W and Tl;
- Group IA: Se and Te;
- Group II: Mo;
- Group III: Be, Tl, Ce, Ti, Th, Zr, V, and U;
- Group VI: Li

Systematic separation of cations into analytical groups followed by identification of individual cations.

2. Determination of chemical constituents in ore samples like nichrome, bronze,

**References**

1. V.V.Ramanujam, Inorganic Semimicro qualitative analysis, National Publishing company, Madras, 1974
2. A. I. Vogel, "Quantitative Inorganic Analysis", ELBS, 3rd Edition, 1971.
3. Vogel's Text book of Inorganic Qualitative Analysis, 4th Ed, ELBS, London, 1974

Mapping of Bloom's Taxonomy with Course Outcome					
	CO1	CO2	CO3	CO4	CO5
K1: Remembering	X	X	X	X	X
K2: Understanding	X	X	X	X	X
K3: Applying	X	X	X	X	X
K4: Analyzing				X	X
K5: Evaluating					X
K6: Creating					X

**SEMESTER –III**  
**PGC 5601**

**Research Methodology Lab**

**10 hr/ 6 cr**

**Course Objectives:**

This course will consider the application of a number of principles as applied to chemical research. This will be achieved by placing students in active research groups in the discipline of chemistry and providing them with the opportunity to carry out research activities.

**Course Outcome:**

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

1. Assess the sources of information related to research
2. Utilize OHP and Power point presentation
3. Acquire the wide knowledge of instrumental analysis
4. Perform computer assisted analysis of data
5. Apply search engine and software tools in research

Students will do the experiments and project work on a title approved by the respective project supervisor. Students will maintain daily records and present oral reports while doing project preparation. All the above process will be duly assessed by the project supervisor. They will submit the collection of research article at the end of the semester.

**Component I - Practical**

1. Multistage organic synthesis
2. Purification & recrystallization techniques
3. Characterisation of compounds using UV-Vis, IR, fluorescence
4. Electrochemical study of inorganic compounds
5. Determination of the formula of a complex by spectrometry
6. Preparation and study of a super conductor
7. Thermodynamics of denaturation of bovine serum albumin  
(Fluorescence spectra)
8. Intermolecular H-bonding in benzyl alcohol using IR spectroscopy
9. Determination of the formation constant of iron(III)salicylate complex

**Component II- Project**

**Evaluation**

Presentation – seminar 25 marks (collective evaluation from all guides)

Project progress (includes 9 experiments) 75 marks from guide

Mapping of Bloom's Taxonomy with Course Outcome					
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K2: Understanding	X	X	X	X	X
K3: Applying	X	X		X	X
K4: Analyzing	X			X	
K5: Evaluating	X			X	
K6: Creating				X	

**Curriculum**  
**for**  
**Second Year M.Sc Chemistry (AIDED) Programme**  
(For those who were admitted from the academic year 2018-2019 onwards)

**SEMESTER IV**



Since 1881

**Postgraduate Department of Chemistry**  
**The American College**  
(An Autonomous Institution Affiliated to Madurai Kamaraj University)  
**Madurai, Tamilnadu, INDIA**

**Course Objectives:**

This is the fourth of the four semester sequential course in organic chemistry. This course deals with retrosynthesis, biologically important steroids and proteins, medicinal chemistry and supramolecular chemistry.

**Course Outcome:**

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

1. Identify various synthons, synthetic equivalents and design a probable synthetic strategy in disconnection of a target molecule.
2. Apply the concepts of retrosynthesis to identify selectivity in synthesis and assess various synthons for effective retrosynthetic approach.
3. Elucidate the structure of steroidal molecules and analyze the structures and functions of proteins and nucleic acids.
4. Explain the various concepts of medicinal chemistry in designing a drug.
5. Analyze the potential applications of various supramolecules and apply green chemistry to organic synthesis.

**UNIT-I : Retrosynthesis-I**

Synthesis – types of synthesis – rational, irrational, linear, convergent, partial, total and biosynthesis - Synthons and types – synthetic equivalent – principles of disconnections in aromatic Target molecule – Functional group interconversion – order of events – guidelines to a good disconnection – one group and two group C – X disconnection and synthetic strategies – one group C-C disconnections in carbonyl compounds – two group disconnections I – Diels-Alder reaction – two group disconnections II : 1,2-, 1,3-, 1,4-, 1,5- and 1,6- difunctional disconnections and strategies.

**UNIT-II : Retrosynthesis-II**

Chemoselectivity – Stereoselectivity – Regioselectivity — Use of aliphatic nitro compounds in organic synthesis – a high light on the use of acetylenes in the synthetic chemistry – amine synthesis – alkene synthesis – Protection and deprotection of groups: alcohols, diols, amine, acids, aldehydes and ketones – Strategy of ring synthesis – small rings such as 3 and 4 membered rings - Retrosynthetic analysis of simple and complex organic molecules – Ferruginol,  $\alpha$ -Bisabolene, Trisporic acid and multistriatin.

**UNIT-III : Steroids, Proteins and Nucleic acids**

Steroids – Basic skeleton – Isolation – Structure determination – Structure of cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progesterone.

Amino acids – Peptides – Proteins, Structure and function conformations of polypeptides – Ramachandran Plot -Peptide synthesis

Nucleotides and Nucleosides – laboratory synthesis of nucleotides and nucleosides – RNA and protein synthesis – Replication-Genetic code – DNA and determining the base sequence of DNA

**UNIT-IV : Medicinal Chemistry**

Drug design – Introduction – Analoges and Prodrugs – Concept of Lead – Factors governing Drug design – Rational approach to drug design– Isosterism and Bio-isosterism – Biopharmaceutical properties of drug substances –Functional groups as binding groups – pharmacophore – Quantitative Structure Activity Relationships –Computer aided drug design – A broad outline of different types of drugs based on pharmacology and their representative examples Host-guest chemistry – Biomimetic chemistry– Proximity effect – molecular adaptation – Transition state analogs – antibodies as enzymes – Suicide enzyme inactivators Molecular recognition and drug design.

## UNIT-V : Supramolecular and Green Chemistry

Introduction to supramolecular chemistry – physical and chemical characteristics of supramolecules - self assembly into mono and multilayers – Structure, reactions and applications- Crown ethers,  $\beta$  - cyclodextrin, Clays, Zeolites, Dendrimers & Fullerenes.

Green chemistry-12 principles-solvent free reactions-microwave assisted reactions-role of ionic liquids ([bmim][BF<sub>4</sub>])- super critical fluids (ScCO<sub>2</sub>)

### References:

1. Futhrhop, Penzlin, Organic synthesis concepts, Methods and Starting materials, Verlag chemie, 1983.
2. Stuart Warren, Organic Synthesis: The Disconnection Approach, John Wiley and Sons, 1992.
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7. I.L. Finar, Organic Chemistry, Vol. II, ELBS, 5<sup>th</sup> edition.
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9. Graham Patrick, Medicinal Chemistry, BIOS Scientific Publishers Ltd., U.K.
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15. S. Zing and Zimmerman, Dendrimers – Structure, properties and applications Chemical Reviews, 1667 – 1698, 1999.
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Mapping of Bloom's Taxonomy with Course Outcome					
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K1: Remembering	X	X	X	X	X
K2: Understanding	X	X	X	X	X
K3: Applying	X	X	X		X
K4: Analyzing	X	X	X		X
K5: Evaluating	X	X			
K6: Creating	X				

**Course Objectives:**

This course attempts to present an overall view of various heteroatom ring systems, their synthesis and reactivity will be discussed. Polymers of such systems and their technological application will also be introduced. It also includes the metal clusters and inorganic photochemistry. Principles and applications of various analytical techniques will also be discussed.

**Course Outcome:**

After completion of the course the students will be able to:

1. Formulate synthetic routes and infer the structure of boron compounds
2. Classify Si-O, P-O & P-S systems and relate the structure with properties
3. Explain the synthesis, reactions and bonding properties of P-N and S-N heterocycles and polymers
4. Establish the structural implications of metal clusters and describe the photochemistry of coordination compounds
5. Analyze the thermal data and evaluate the analytical data

**UNIT – I: CHEMISTRY OF BORON HETEROSYSTEMS**

Boron and multicentered bonds – types of bonds – diborane – tetraborane – synthesis – chemical reactions – structure and bonding – higher boranes –  $B_{10}H_{14}$  – bonding – classification by Wade's rule – topological structure – styx number – structural studies by IR and NMR – carboranes – preparation, properties – metallocarboranes – monocarboranes – carboranes with more than two cage carbon atoms.

**B-N systems:** borazines – comparison with benzene – N and B substituted borazines – hydrolytic stability – B-O systems – borates.

**UNIT – II: Si-O, P-O, P-S SYSTEMS**

**Silicates:** classification – asbestos minerals – Zeolites – organosilicon compounds – silicone polymer – types – preparation – uses – siloxanes – reactions – polymerisation of cyclosiloxane – mechanism – factors influencing polymerization.

**P-S rings and cages:** synthesis and reactions – P-O heterocyclic compounds – preparation – reactions – linear & cyclic phosphates ( $Na_2HPO_4$ ,  $NaH_2PO_4$ ,  $Na_3P_3O_9$ ) – inter conversions of various phosphates – applications – P-O compounds – preparation and reactions.

**UNIT – III: P-N and S-N HETEROSYSTEMS**

**P-N system:**  $N_3P_3Cl_6$ ,  $N_4P_4Cl_8$ ,  $(NPCl_2)_x$  – Synthesis, uses, theories of bonding, electronic structure and aromaticity – reactions: hydrolysis, aminolysis, metathetical reactions, organometallic reagents, Friedel-Crafts substitutions, rearrangements

**S-N heteroatom systems:** bonding – Huckel's rule –  $S_4N_4$ : preparation, structure (Banister and Mingos models), properties –  $S_4N_3Cl$ ,  $S_3N_2Cl_2$ ,  $S_4N_4O_4$ : preparation, structure, properties –  $S_4N_2$ : preparation, structure determination –  $(SN)_x$ : preparation, structure, properties

**UNIT-IV: METAL CLUSTER COMPOUNDS AND INORGANIC PHOTOCHEMISTRY**

Metal atom clusters – high nuclearity carbonyl clusters – lower halide clusters – isoelectronic and isolobal analogy – structure implications – their synthetic utility – electron counting schemes – capping rule – compounds with M-M multiple bonds

Basic photochemical process – Photosubstitution – Adamson's rule – photoredox – ligand photo reaction – photo induced cleavage of M-M bonds-evidences– ligand field photochemistry of  $d^3$ ,  $d^6$  complexes – photochemical cleavage of water - solar energy conversion

## UNIT-V: ANALYTICAL TECHNIQUES

**Thermal analysis:** TGA, DTA, DSC – principle, instrumentation, factors affecting - applications.

**Evaluation of data:** Significant figures – accuracy – precision – Gaussian distribution – Poisson distribution – confidence levels – tests of significance - F test, student t test – least square analysis – correlation coefficient – criteria for rejection of data- Q test.

### References:

1. H.R.Allock, Phosphorus – Nitrogen compounds, Academic Press, New York, 1967.
2. N.H.Ray, Inorganic Polymers, Academic Press, New York, 1978.
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Mapping of Bloom's Taxonomy with Course Outcome					
	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5
	CO1	CO2	CO3	CO4	CO5
K1: Remembering	X	X	X	X	X
K2: Understanding	X	X	X	X	X
K3: Applying	X	X	X	X	X
K4: Analyzing	X			X	X
K5: Evaluating	X				
K6: Creating					



**Course objectives:**

The learners should be able to link microscopic properties of matter and its bulk properties, predict the population of states in systems at thermal equilibrium, acquire skills in understanding catalysis and adsorption phenomena, acquire analytical skills in understanding polymerization using latest techniques and explore the frontiers of nanoscience.

**Course outcome:**

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

1. Assess partition functions and relate them with thermodynamic functions.
2. Compare the various statistics and their implication to different state of molecules.
3. Examine the kinetics and catalysis of reactions in solution.
4. Deduce the parameters involved in different types of polymerization and explain the techniques for molecular weight determination.
5. Compare the types of sensors and the associated physical effects involved in signal transduction.

**UNIT – I: STATISTICAL THERMODYNAMICS – I**

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging, Canonical, Grand canonical and microcanonical ensembles, corresponding distribution laws. Maxwell-Boltzmann statistics – Partition functions – thermodynamic properties from partition function – translational, rotational, vibrational and electronic partition functions. Partition function and equilibrium constant.

**UNIT – II: STATISTICAL THERMODYNAMICS – II**

Quantum statistics – Fermi-Dirac and Bose-Einstein statistics – photon gas, Bose-Einstein condensation, degeneracy and Bose-Einstein condensation, application to liquid He. Electron gas, degeneracy and electron gas. Heat capacities of diatomic gases. Einstein and Debye's theory of heat capacity of solids – paramagnetism – population inversion – negative Kelvin temperature.

**UNIT – III: CHEMICAL KINETICS – II AND SURFACE CHEMISTRY**

Homogeneous catalysis – acid-base catalysis, acidity function – Michaelis-Menten kinetics. Fast reaction techniques – chemical relaxation methods, T-jump and P-jump methods, ultrasonic absorption techniques, reaction in a flow system, continuous and stopped flow, shock wave tube method. Micelles – surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration, factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization – reverse micelles.

Physisorption and Chemisorption – Langmuir and BET adsorption – Gibbs adsorption isotherm – insoluble surface films – electrokinetic phenomena – zeta potential – Heterogeneous catalysis – reactions and their kinetics.

**UNIT – IV: POLYMER CHEMISTRY**

Introduction – Classification of polymers – chemistry of polymerization – chain – Free-Radical Polymerisation – Ionic polymerization – Coordination polymerization – Step polymerization – Polycondensation – Polyaddition polymerization – Ring-opening polymerization – polymerization techniques. Copolymerisation – Ionic – free radical – copolycondensation.

Kinetics of polymerization – Free-Radical chain polymerization – cationic polymerization – Anionic polymerization – polycondensation. Measurement of molecular weight and size. End-group analysis – colligative property measurement – light scattering – ultracentrifugation – solution viscosity and molecular size – gel permeation chromatography – polyelectrolysis.

## UNIT – V: NANOSENSORS

Micro & nanosensors, Active and Passive sensors – Static characteristic - Accuracy, offset and linearity – Dynamic characteristics - First and second order sensors-Physical effects involved in signal transduction- Photoelectric effect – Photo dielectric effect – Photoluminescence effect – Electroluminescence effect – Hall effect – Thermoelectric effect – Piezoresistive effect – Piezoelectric effect – Pyroelectric effect – Magnetomechanical effect (magnetostriction).

Selectivity of Potentiometric Sensor - Measurement with Potentiometric Sensors- Selectivity of Amperometric Sensors – Measurement with Amperometric Sensors - Classes of Electrochemical Biosensors. Sensors with Thermistors and Peltistors - Pyroelectric Sensors- Fibre Sensors Without Chemical Receptors & with chemical receptors.

### References:

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Mapping of Bloom’s Taxonomy with Course Outcome					
	Unit-I	Unit-II	Unit-III	Unit-IV	Unit-V
	CO1	CO2	CO3	CO4	CO5
K1: Remembering	X	X	X	X	X
K2: Understanding	X	X	X	X	X
K3: Applying	X	X	X	X	X
K4: Analyzing	X	X	X	X	X
K5: Evaluating	X	X		X	X
K6: Creating					

**Course Objectives:**

This is a laboratory course that deals with the principles and various analytical methods of quantitative analysis of cations present in a mixture.

**Course Outcome:**

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

1. Summarize the principle of calibration and standards
2. Perform calibration of apparatus
3. Develop analytical skill in the field of estimation of cations in mixture
4. Highlight the principle of methods of cation estimation
5. Design methods to analyze industrial effluents, antique pieces and environmental samples

**Component 1:**

Calibration of apparatus – Burette, Pipette, Volumetric flasks

Assessment of errors in apparatus and distribution

**Component 2:**

1. Estimation of Cu(II) – Iodometry & Gravimetric method
2. Estimation of Cu(II) and Ni(II) – Iodometry & Gravimetric
3. Estimation of Cu(II) and Ni(II) – Spectrophotometric
4. Estimation of Fe(II) and Fe(III) – Reduction & Redox titration
5. Estimation of Cu(II) and Zn(II) – Acidimetry with glass pH electrode/potentiometry
6. Estimation of Ca(II) and Mg(II) – Complexometric with pH control
7. Estimation of Ni(II) and Zn(II) – Complexometric/kinetic control/potentiometric
8. Estimation of Cu(II) and Ca(II) – Iodometry / reduction/ Complexometry

**Component 3:**

1. Determination of total hardness of water
2. Determination of Mn content in steel
3. Determination of Cu content in brass

**REFERENCES**

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Mapping of Bloom's Taxonomy with Course Outcome					
	CO1	CO2	CO3	CO4	CO5
K1: Remembering	X	X	X	X	X
K2: Understanding	X	X	X	X	X
K3: Applying	X	X	X	X	X
K4: Analyzing		X	X	X	X
K5: Evaluating					X
K6: Creating					

**SEMESTER –IV****PGC 5602****PROJECT****10 hr/ 6 cr****Course objectives:**

This course is designed to reinforce the concepts with analytical techniques. It will provide a platform for students to have a hands-on experience with instruments and present a report on a research topic.

**Course outcome:**

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

1. Design, conduct, analyze and interpret results of an experiment, and effectively communicate these in written reports
2. Develop interdisciplinary solutions to a variety of chemical problems.
3. Communicate effectively in a variety of forms.
4. Use terminology appropriate to the field of study correctly and contextually.
5. Extend knowledge and understanding of a variety of chemical concepts in a range of contexts.

Students will do the project work on a title approved by the respective project supervisor. Students will maintain daily records and present oral reports while doing the project. All the above process will be duly assessed by the project supervisor. They will submit the thesis at the end of the semester.

**Evaluation**

Project presentation	25 marks (collective evaluation from all guides)
Project progress	50 marks from guide
Thesis	25 marks from guide

Mapping of Bloom's Taxonomy with Course Outcome					
	CO1	CO2	CO3	CO4	CO5
K1: Remembering	X	X	X	X	X
K2: Understanding	X	X	X	X	X
K3: Applying	X	X	X	X	X
K4: Analyzing	X	X			X
K5: Evaluating	X	X			X
K6: Creating	X	X			X