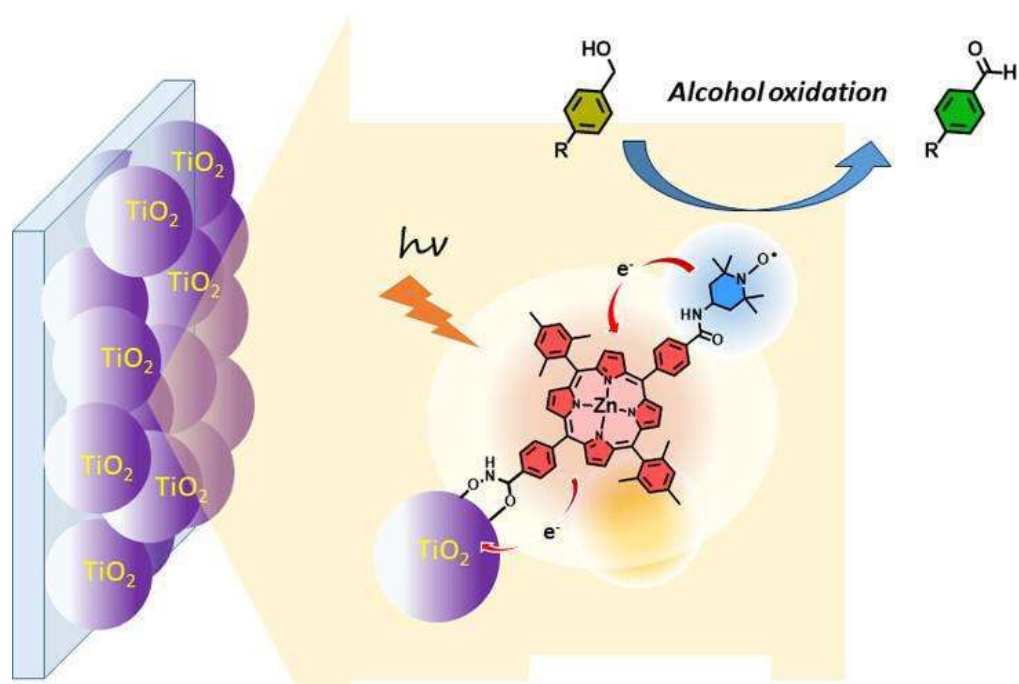


# Integrated M.Sc. Chemistry (CBCS) SYLLABUS



Department of Chemistry  
Central University of Tamil Nadu  
Thiruvavur 610 005  
2021

## VISION

The Department envision establishing itself as a place of excellence for chemistry education and research programmes in the nation.

We envision a place of excellence in chemistry education (Learning - Understanding) and research (Product development - knowledge dissemination) for the development of our nation.

## MISSION

**M1:** To bridge the gap between academia and industry by regularly updating the curriculum on par with recent developments in science and encourage to do inhouse projects

**M2:** To educate and invoke the students to deliver their maximum outputs in competitive examinations (NET & GATE) and meet industrial competences.

**M3:** To develop chemists with excellent analytical & synthetic skills, we enrich the curriculum with more laboratory components and facilitate industrial visits/internships in Chemical companies & National Laboratories.

## Programme Educational Objectives (PEOs)

The Integrated M.Sc. (IMSc) Chemistry programme will enable the student to

**PEO1:** seamlessly integrate knowledge from other disciplines such as Mathematics, Physics and Life-sciences to enable interdisciplinary and multidisciplinary research.

**PEO2:** have societal, health, safety, and cultural issues relevant to the science practices and provide a strong foundation for acquiring advanced knowledge in chemistry

**PEO3:** acquire critical thinking supported by advanced analytical skills to address chemistry related problems.

**PEO4:** demonstrate the ability to perform accurate quantitative measurements with an understanding of the theory and use of sophisticated instruments, analyse and interpret.

**PEO5:** enhance skills for employability through activities, such as, seminar, communication skills, industrial visit, internship, and research project dissertation.

Mission	PEO1	PEO2	PEO3	PEO4	PEO5
M1	2	2	3	3	3
M2	3	2	2	2	3
M3	2	3	3	3	3

## Graduate Attributes

- **Disciplinary Knowledge:** Content and pedagogical knowledge synchronised with the curriculum frameworks and policies
- **Communication Skills:** Possess clarity in conveying the ideas
- **Critical Thinking:** Capacity to apply analytical thought in the teaching and learning process
- **Problem Solving:** Participate in the educational problem solving and applying the knowledge in the day-to-day professional endeavours.

- Cooperation: Appreciate collaboration and cooperation among stakeholders of education.
- ICT Skills: Selecting and integrating appropriate ICT skills for professional development.
- Ethics: Doing what is right to society
- Self-Directed Learning: Developing autonomy and self-regulation in teaching learning and professional development.
- Reasoning: Ability to interpret and draw the conclusion from qualitative/quantitative data with open-mindedness
- Creativity: Ability to produce new ideas
- Societal and Environmental Concern: Performing an act or solving a problem with respect to societal and environmental concern
- Lifelong Learning: Understands the need for learning and practices it throughout life

### Programme Outcomes (POs)

On successful completion of integrated M.Sc programme, the student will be able to

**PO1:** Think critically and analyse problems.

**PO2:** Prepare and present scientific and technical information resulting from laboratory outputs.

**PO3:** Design methodologies, analyse, and evaluate innovative scientific research problems.

**PO4:** Pursue higher education / become an employee / entrepreneur.

**PO5:** Work independently as well as in a team.

POs	PEO1	PEO2	PEO3	PEO4	PEO5
PO1	3	3	3	3	3
PO2	3	2	3	3	2
PO3	2	3	3	2	2
PO4	3	3	3	3	3
PO5	3	2	2	3	3

### Programme Specific Outcomes (PSOs)

Upon successful completion of integrated M.Sc. Chemistry programme, the student will be able to

**PSO1:** Acquire the knowledge of fundamental chemistry concepts and recent advancement in the scientific field.

**PSO2:** Understand the features of molecules in organic /inorganic/physical domain

**PSO3:** Develop computational and experimental skills to explore molecular level phenomena.

**PSO4:** Apply technical skill in a sophisticated laboratory environment & secure challenging positions in Industry & Academics.

**PSO5:** Enhance employability through laboratory activities, solving problems and co-curricular activities

## iMSc Chemistry- Credit Distribution

Sem ester		Title of the Course	Nature of the course	Credit
1	CHE1011	General Chemistry	T	3
1	CHE1012	General Chemistry Laboratory	P	2
1		Second Major	T	3
1		Second Major Laboratory	P	2
1		Third Major	T	3
1		Third Major Laboratory	P	2
1		*****Ability Enhancement Course *****	AECC	2
1		English – 1	AECC	3
2	CHE1021	Physical Chemistry I	T	3
2	CHE1022	Physical Chemistry Laboratory I	P	2
2		Second Major	T	3
2		Second Major Laboratory	P	2
2		Third Major	T	3
2		Third Major Laboratory	P	2
2		*****Ability Enhancement Course *****	AECC	2
2		English – 2	AECC	3
3	CHE1031	Inorganic Chemistry I	T	3
3	CHE1032	Inorganic Chemistry Laboratory I	P	2
3		Second Major	T	3
3		Second Major Laboratory	P	2
3		Third Major	T	3
3		Third Major Laboratory	P	2
3		*****Ability Enhancement Course *****	AECC	2
3		Language – 1	AECC	3
4	CHE1041	Organic Chemistry I	T	3
4	CHE1042	Organic Chemistry Laboratory I	P	2
4		Second Major	T	3
4		Second Major Laboratory	P	2
4		Third Major	T	3
4		Third Major Laboratory	P	2
4		*****Ability Enhancement Course *****	AECC	2
4		Language – 2	AECC	3
5	CHE1051	Analytical Methods in Chemistry	DSE-T	4
5	CHE1052	Acid-bases, redox reactions, s- and p- block elements	DSE-T	4
5	CHE1053	Organic Reaction Mechanisms & Heterocyclic compounds	DSE-T	4

5	CHE1054	Physical States of Matter & Photochemistry	DSE-T	4
5	CHE1055	Analytical & Inorganic Chemistry Laboratory I	DSE-P	2
5	CHE1056	Organic Chemistry Laboratory II	DSE-P	2
5	CHE1057	Physical Chemistry Laboratory II	DSE-P	2
5		*****Skill Enhancement Course*****	SEC	2
6	CHE1061	Nuclear, Basic Organometallic and Bioinorganic Chemistry	DSE-T	4
6	CHE1062	Reaction Mechanisms and Natural Products Chemistry	DSE-T	4
6	CHE1063	Quantum Chemistry and Molecular Spectroscopy	DSE-T	4
6	CHE1064	Analytical & Inorganic Chemistry Laboratory II	DSE-P	2
6	CHE1065	Organic Chemistry Laboratory III	DSE-P	2
6	CHE1066	Physical Chemistry Laboratory III	DSE-P	2
6		*****Skill Enhancement Course*****	SEC	2
6	CHE1067	#### Project (for students opting exit)**	P	6
7	CHE1071	Solid State, Main Group and Coordination Chemistry	T	4
7	CHE1072	Physical Organic Chemistry & Aromatic Compounds	T	4
7	CHE1073	Chemical Kinetics and Group Theory	T	4
7		*****Subject Selective Elective*****	E	4
7	CHE1074	Advanced Organic Chemistry Laboratory	P	4
8	CHE1081	Advanced Organometallic and Bioinorganic Chemistry	T	4
8	CHE1082	Organic Photochemistry and Rearrangements	T	4
8	CHE1083	Advanced Quantum Mechanics & Molecular Spectroscopy	T	4
8	CHE1084	Physical Methods in Chemistry I	T	4
8	CHE1085	Advanced Physical Chemistry Laboratory	P	4
9	CHE1091	Physical methods in Chemistry II	T	4
9	CHE1092	Reagents & Synthetic Strategies in Organic Chemistry	T	4
9	CHE1093	Thermodynamics (Classical/statistical) & Electrochemistry	T	4
9		*****Subject Selective Elective*****	E	4
9	CHE1094	Advanced Inorganic Chemistry Laboratory	P	4
10	CHE1101	Research Project	P	12

**Total:** 124 + 6 = 130 credits for B.Sc (Exit) option candidates. Those who opt for the exit option should give in writing to the department with an endorsement from the concerned parent at the end of second year (fourth semester).

Total: 196 credits for iMSc Candidates

The I.MSc students with Maths background will be given Maths and Physics as other majors, whereas i.MSc students with Life-Science / Biology background will be given Physics and Life-Science as other major subjects.

**Semester I**  
**CHE1011 - General Chemistry**

**Credits: 3**  
**Theory**

Course Outcomes		Level
CO-1	Understand the basic concepts of atomic structure and chemical bonding	Understand
CO-2	Analyze the concept of inorganic and organic chemistry	Analyze
CO-3	Assess the atomic structures, chemical bonding and their kinetics	Remember
CO-4	Predict various isomerism and nomenclature methods in stereochemistry	Remember

**Atomic Structure:**

Review of Bohr's theory and its limitations, dual behaviour of matter and radiation, de Broglie's relation, Heisenberg Uncertainty principle. Hydrogen atom spectra. Need of a new approach to Atomic structure.

Introduction to Quantum mechanics: Time independent Schrodinger equation and meaning of various terms in it. Significance of  $\psi$  and  $\psi^2$ , Schrödinger equation for hydrogen atom. Radial and angular parts of the hydrogenic wavefunctions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals (Only graphical representation). Radial and angular nodes and their significance. Radial distribution functions and the concept of the most probable distance with special reference to 1s and 2s atomic orbitals. Discovery of spin, spin quantum number (s) and magnetic spin quantum number ( $m_s$ ). Significance of quantum numbers, orbital angular momentum and quantum numbers  $m_l$  and  $m_s$ . Shapes of s, p and d atomic orbitals, nodal planes.

Rules for filling electrons in various orbitals, Electronic configurations of the atoms. Stability of half-filled and completely filled orbitals, concept of exchange energy. Relative energies of atomic orbitals, Anomalous electronic configurations.

**Chemical Bonding and Molecular Structure:**

Ionic Bonding: General characteristics of ionic bonding. Energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and solubility of ionic compounds. Statement of Born-Landé equation for calculation of lattice energy, Born-Haber cycle and its applications, polarizing power and polarizability. Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

**Fundamentals of Organic Chemistry:**

Physical Effects, Electronic Displacements: Inductive Effect, Electromeric Effect, Resonance and Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis. Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles. Reactive Intermediates: Carbocations, Carbanions and free radicals. Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values. Aromaticity: Benzenoids and Hückel's rule.

**Organic Stereochemistry:**

Conformations with respect to ethane, butane and cyclohexane. Interconversion of Wedge Formula, Newman, Sawhorse and Fischer representations. Concept of chirality (upto two carbon atoms). Configuration: Geometrical and Optical isomerism; Enantiomerism, Diastereomerism and Meso compounds). Threo and erythro; D and L; cis – trans nomenclature; CIP Rules: R/ S (for upto 2 chiral carbon atoms) and E / Z Nomenclature (for upto two C=C systems).

**Chemical Energetics:**

Review of thermodynamics and the Laws of Thermodynamics. Important principles and definitions of thermochemistry. Concept of standard state and standard enthalpies of formations, integral and differential enthalpies of solution and dilution. Calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data. Variation of enthalpy of a reaction with temperature – Kirchhoff's equation. Statement of Third Law of thermodynamics and calculation of absolute entropies of substances.

**Ionic Equilibria:**

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions. Solubility and solubility product of sparingly soluble salts-applications of solubility product principle.

**Chemical Kinetics:**

The concept of reaction rates. Effect of temperature, pressure, catalyst and other factors on reaction rates. Order and molecularity of a reaction. Derivation of integrated rate equations for zero, first and second order reactions (both for equal and unequal concentrations of reactants). Half-life of a reaction. General methods for determination of order of a reaction. Concept of activation energy and its calculation from Arrhenius equation. Theories of Reaction Rates: Collision theory and Activated Complex theory of bimolecular reactions. Comparison of the two theories (qualitative treatment only).

**Reference Books**

1. D. D. Ebbing, General Chemistry, 10<sup>th</sup>edn, Cengage Learning India Pvt. Ltd.; Tenth edition, **2013**.
2. J.D. Lee, Concise Inorganic Chemistry, Wiley, 5<sup>th</sup> edn., **2016**.
3. R. P. Rastogi, R. R. Misra, An Introduction to Chemical Thermodynamics, 6th edn., Vikas Pub. Pvt. Ltd. **2003**.
4. P. Atkins and J Paula, The elements of Physical chemistry, 7th edn., Oxford University Press, **2017**.
5. K. K. Sharma, L. K. Sharma, A Textbook of Physical Chemistry, 4th edn, Vikas publishing House, **2008**.
6. B. R. Puri, L. R. Sharma, M. S. Pathania, Elements of Physical chemistry, Vishal Pub. Co. Jalandhar, **2017**.
7. G. K. Vemulapalli, Physical Chemistry, Prentice-Hall of India Pvt. Ltd. **1997**.

- K. J. Laidler, Chemical kinetics 3rd edn, Pearson education, **2004**.
- Graham Solomons, T. W. Fryhle, C. B. Snyder, S. A., Organic Chemistry, 12th edn, Wiley, **2016**.
- J.E. Mc Murry, Fundamentals of Organic Chemistry, 7th edn, Cengage Learning India Edition, **2013**.
- P.Sykes, A Guidebook to Mechanism in Organic Chemistry, 6<sup>th</sup> Ed., Orient Longman, New Delhi, **1988**.
- E.L. Eliel, Stereochemistry of Carbon Compounds, Tata McGraw Hill education, **2013**.
- I.L. Finar, Organic Chemistry (Vol. I & II), Vol I, 6th edn, Pearson Education, **2002**.
- R.T. Morrison, R.N. Boyd, Organic Chemistry, 7th edn, Pearson Education, **2010**.

#### Further reading:

- J. Rajaram and J. C. Kuriakose, Thermodynamics, Shoban Lal Nagin Chand & Co.,**1986**.
- H. Kuhn and H. D. Fosterling, Principles of Physical Chemistry, 2<sup>nd</sup> Ed., John Wiley & Sons, **2009**.
- W. J. Moore, Basic Physical Chemistry, Orient Longman, **1963**.
- F. A. Alberty and R. J. Silby, Physical Chemistry, 4<sup>th</sup> Ed., John Wiley, **2004**.
- G. M. Barrow, Physical Chemistry, 5th edn., Tata McGraw Hill, **2007**.
- G. W. Castellan, Physical Chemistry, 3rd edn, Narosa Publishing House, New Delhi, **2004**.
- J.Clayden, N.Greeves, S.Warren. Organic Chemistry, 2nd edn, Oxford University Press, **2014**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	1	1	1	1	1
CO2	2	1	2	1	1
CO3	3	1	2	1	1
CO4	3	1	2	1	1

#### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
Total	25	25	25	25	100

#### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20

Attendance	2	1	1	1	5
Total	12	9	9	10	40

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)	-	5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
Total	10	14	15	21	60

### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	
Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Structuring (30 %)	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	
Drafting skill (30 %)	Good language & < 2 % Plagiarism	Good language & < 5 % Plagiarism	< 10 % Plagiarism	> 10 % Plagiarism	

### MODEL QUESTION PAPER

**CHE1011 - General Chemistry – I**

**Duration: 3 Hours**

**Max. Marks: 60**

**PART A**

**ANSWER THE FOLLOWING QUESTIONS**

**(10 x 1 = 10)**

1. Is half-filled orbitals a direct application of Hund's rule? Why?
2. Chemical bond implies
  - (a) repulsion, (b) attraction, (c) attraction and repulsion,
  - (d) attraction and repulsion balanced at particular distance

**PART- B**

**ANSWER ANY FIVE QUESTIONS**

**(5 x 3 = 15)**

11. How to calculate activation energy ( $E_a$ ) for exothermic and endothermic reactions?
12. Write about the polarising power and polarizability.

**PART-C**

**ANSWER ALL THE QUESTIONS**

**(5 x 7 = 35)**

18. a) (i) Explain the time independent wave equation.  
(ii) What is the de Broglie wavelength of an molecule travelling at half the speed of the given speed (C) (mass of molecule =  $3.4 \times 10^{-27}$  kg,  $C = 3400 \text{ ms}^{-1}$ )

(OR)

18. b) (i) Explain nodal lobes and nodal planes are present in s, p, and d orbital.  
(ii) How to calculate orbital angular momentum and spin quantum numbers for anelectron of spin in clockwise direction and present in p-orbital.

**Semester I**  
**CHE1012 -General Chemistry Laboratory**

**Credits: 2**

**Practical**

Course Outcomes		Level
CO-1	Estimate heat transfer of various reactions and thermodynamic parameters	Analyze
CO-2	Use pH measurements for assessing the acidic and basic properties	Apply
CO-3	Prepare buffer solutions and standards	Apply
CO-4	Estimate the ionic equilibrium in a given system	Analyze

**Thermochemistry:**

1. Determination of heat capacity of calorimeter for different volumes.
2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
3. Determination of enthalpy of ionization of acetic acid.
4. Determination of integral enthalpy of solution of salts (KNO<sub>3</sub>, NH<sub>4</sub>Cl).
5. Determination of enthalpy of hydration of copper sulphate.
6. Study of the solubility of benzoic acid in water and determination of  $\Delta H$ .

**Ionic Equilibria:**

1. Measurement of pH of different solutions like aerated drinks, fruit juices, shampoos and soaps using pH-meter.
2. Preparation of buffer solutions:
  - a) Sodium acetate-acetic acid
  - b) Ammonium chloride-ammonium hydroxide
3. Measurement of the pH of buffer solutions and comparison of the values with theoretical values.

**Reference books**

1. B. Viswanathan, Practical Physical chemistry, Viva Pub., **2005**.
2. Saroj Kumar and Naba Kumar, Physical Chemistry Practical, New Central Book Agency, **2012**.
3. A.M. James, F.E. Prichard Practical Physical Chemistry Paperback, **1974**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	3	2	1	3
CO2	1	3	1	1	3
CO3	2	3	2	1	3
CO4	2	3	3	2	3

## Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
<b>Internal</b>	15	15	15	15	60
<b>External</b>	10	10	10	10	40
<b>Total</b>	25	25	25	25	100

## Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Punctuality	3	3	3	3	12
Experiment skill	3	3	3	3	12
Performance in Lab	3	3	3	3	12
Maintenance of Observation Records	3	3	3	3	12
Attendance	3	3	3	3	12
<b>Total</b>	15	15	15	15	60

## Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Viva - 01 & 02	5	5	5	5	20
Skill Evaluation	3	3	3	3	12
Record	2	2	2	2	8
<b>Total</b>	10	10	10	10	40

## Rubric for Internal Assessment

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Punctuality and safety measures	Punctual in coming to the lab and carrying essential safety things	Less punctual and missing any safety things	Ignorant in attending practical and missing 50% safety things	Not attending and no safety things	All
Knowledge about the experiment	Exceptional knowledge about experiment	Considerable knowledge about the experiment	Minimal knowledge about the experiment	Not attended	
Handling of apparatus and recording of observation	Accurate handling of apparatus & Accurate, precise and	Less proper but careful handling of apparatus &	Proper but careless handling of	Not attended	

	<b>appropriate reporting and recording the results in SI units</b>	<b>Wrong but appropriate reporting and use of SI units</b>	<b>apparatus &amp; Incorrect way of recording observation</b>		
<b>Maintenance of record book</b>	<b>Perfect presentation of record in terms of completeness, neatness, well maintenance and sticking to the dead line of submission</b>	<b>Completing and fine maintenance of record. Adhering to the dead line</b>	<b>Incomplete record</b>	<b>Not submitting</b>	

**Semester II**  
**CHE1021 - Physical Chemistry I**

**Credits: 3**  
**Theory**

Course Outcomes		Level
CO-1	To acquire basic knowledge of reactions using Chemical Equilibrium concepts.	Remember
CO-2	To identify different types of solutions as a function of C, P, V and T.	Apply
CO-3	To understand the chemical reactions in the batteries, corrosion etc.	Understand
CO-4	To analyze the properties of solutions, cells, etc. to innovate new methodologies	Analyze

**Chemical Equilibrium:** Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. Distinction between  $\Delta G$  and  $\Delta G_0$ , Le Chatelier's principle. Relationships between  $K_p$ ,  $K_c$  and  $K_x$  for reactions involving ideal gases.

**Solutions:** Thermodynamics of ideal solutions: Ideal solutions and Raoult's law, deviations from Raoult's law – non-ideal solutions. Vapour pressure-composition and temperature composition curves of ideal and non-ideal solutions. Distillation of solutions. Lever rule. Azeotropes. Partial miscibility of liquids: Critical solution temperature; effect of impurity on partial miscibility of liquids. Immiscibility of liquids- Principle of steam distillation. Nernst distribution law and its applications, solvent extraction.

**Phase Equilibrium:** Phases, components and degrees of freedom of a system, criteria of phase equilibrium. Gibbs Phase Rule and its thermodynamic derivation. Derivation of Clausius – Clapeyron equation and its importance in phase equilibria. Phase diagrams of one-component systems (water and sulphur) and two component systems involving eutectics, congruent and incongruent melting points (lead-silver,  $\text{FeCl}_3\text{-H}_2\text{O}$  and Na-K only).

**Conductance:** Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Kohlrausch law of independent migration of ions. Transference number and its experimental determination using Hittorf and Moving boundary methods. Ionic mobility. Applications of conductance measurements: determination of degree of ionization of weak electrolyte, solubility and solubility products of sparingly soluble salts, ionic product of water, hydrolysis constant of a salt. Conductometric titrations (only acid-base).

**Electrochemistry:** Reversible and irreversible cells. Concept of EMF of a cell. Measurement of EMF of a cell. Nernst equation and its importance. Types of electrodes. Standard electrode potential. Electrochemical series. Thermodynamics of a reversible cell, calculation of thermodynamic properties:  $\Delta G$ ,  $\Delta H$  and  $\Delta S$  from EMF data. Calculation of equilibrium constant

from EMF data. Concentration cells with transference and without transference. Liquid junction potential and salt bridge. pH determination using hydrogen electrode and quinhydrone electrode. Potentiometric titrations -qualitative treatment (acid-base and oxidation-reduction only). Irreversible electrode processes – overvoltage. Corrosion of metals – forms of corrosion, corrosion monitoring and prevention methods.

### Reference Books

1. G.M. Barrow, Physical Chemistry Tata McGraw-Hill **2007**.
2. G.W. Castellan, Physical Chemistry 4th Ed. Narosa **2004**.
3. J.C. Kotz, P.M. Treichel & J.R. Townsend, General Chemistry Cengage Learning India Pvt. Ltd., New Delhi **2009**.
4. R. P. Rastogi, R. R. Misra, An Introduction to Chemical Thermodynamics, 6th edn., Vikas Pub. Pvt. Ltd. **2003**.
5. B.H. Mahan, University Chemistry 3rd Ed. Narosa **1998**.
6. R.H. Petrucci, General Chemistry 5th Ed. Macmillan Publishing Co.: New York **1985**.
7. B. R. Puri, L. R. Sharma, M. S. Pathania, Elements of Physical chemistry, Vishal Pub. Co. Jalandhar.
8. K. L. Kapoor, A Textbook of Physical Chemistry, Volumes 1, Macmillan India Ltd,
9. P. Atkins and J Paula, The elements of Physical chemistry, 7th edn., Oxford University Press.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	1	2	1	1
CO2	3	1	2	1	1
CO3	2	1	2	1	1
CO4	3	1	3	1	1

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
Total	25	25	25	25	100

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
Total	12	9	9	10	40

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

#### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	
Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

#### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Structuring (30 %)	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

<b>Drafting skill (30 %)</b>	<b>Good language &amp;&lt; 2 % Plagiarism</b>	<b>Good language &amp;&lt; 5 % Plagiarism</b>	<b>&lt; 10 % Plagiarism</b>	<b>&gt; 10 % Plagiarism</b>	
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**MODEL QUESTION PAPER  
CHE1021 PHYSICAL CHEMISTRY-I**

**PART – A**

**ANSWER ANY FIVE QUESTIONS**

**(5 x 2 = 10marks)**

- A dilatometer is an apparatus used to measure -----  
(a) Transition temperature    (b) Triple point    (c) Eutectic point    (d) Melting point
- While determining transport number by Hittorf's method ----- electrodes are used when the electrodes are attackable.  
(a) Silver                            (b) Copper                            (c) Mercury                            (d) Platinum

**PART - B**

**ANSWER ANY FIVE QUESTIONS**

**(5 x 3 = 15marks)**

- (a) Calculate the total vapour pressure in torr for the solution which contains two volatile liquids based on the following information:  
Component 1: Benzene : Volume = 25 mL, Density = 0.877 g/mL,  $p^0 = 70$  torr  
Component 2: Toluene : Volume = 100 mL, Density = 0.866 g/mL,  $p^0 = 20$  torr (2)  
(b) Draw the vapour pressure – composition curve of minimum boiling azeotrope.
- (a) State Kohlrausch's Law. (1)  
(b) The speed ratio of silver and nitrate ions in a solution of  $\text{AgNO}_3$  electrolysed between silver electrode is 0.916. Find the transport number of the two ions. (2)

**Part – C**

Answer ALL the questions

[5 x 7M = 35 Marks]

- A (i) Draw a labelled phase diagram of the water system. Explain clearly the main points of information about the equilibria represented in various areas, along different curves and at various points of the diagram. (5)

(ii) Determine the vapour pressure in mm Hg of a substance at  $45^{\circ}\text{C}$ . If its normal boiling point is  $115^{\circ}\text{C}$  and its enthalpy of vaporization is  $57.9\text{ kJ mol}^{-1}$ . (2)

[OR]

1.B (i) Sketch the phase diagram of  $\text{FeCl}_3\text{-H}_2\text{O}$  system. (2)

(ii) Explain the phase diagram of  $\text{Pb-Ag}$  system and write its salient features. Highlight the Pattinson's process. (5)

**Semester II**  
**CHE1022 - Physical Chemistry Laboratory I**

**Credits: 2**

**Practical**

Course Outcomes		Level
CO-1	To experiment with the basic skills required for wet lab chemistry.	Analyze
CO-2	To apply or correlate the physical chemistry concepts with the experiments.	Apply
CO-3	To identify or perform the appropriate experiments for the measurements of concentration.	Understand
CO-4	To execute solvent extraction process and eutectic experiments	Apply

**Partition Coefficient:**

1. Study the partition of solute in two immiscible liquids
2. Study of the equilibrium of the following reactions by the distribution method:  

$$I_2(aq) + I^-(aq) \rightarrow I_3^-(aq)$$

**Phase equilibria:**

1. Construction of the phase diagram of a binary system (simple eutectic) using cooling curves.
2. Determination of the critical solution temperature and composition of the phenol water system and study of the effect of impurities on it.

**Potentiometry: Perform the following potentiometric titrations:**

1. Strong acid vs. strong base
2. Weak acid vs. strong base

**Conductance: conductometric titrations:**

1. Strong acid vs. strong base
2. Weak acid vs. strong base

**Reference Books**

1. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, **2001**.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Ed. McGraw Hill, **2009**.
3. A.M. James and F.E. Prichard Practical Physical Chemistry Paperback, **1974**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	1	3	2	1	3
CO2	2	3	1	1	3
CO3	2	3	3	1	3
CO4	1	3	2	1	3

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	15	15	15	15	60
External	10	10	10	10	40
<b>Total</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>100</b>

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Punctuality	3	3	3	3	12
Experiment skill	3	3	3	3	12
Performance in Lab	3	3	3	3	12
Maintenance of Observation Records	3	3	3	3	12
Attendance	3	3	3	3	12
<b>Total</b>	<b>15</b>	<b>15</b>	<b>15</b>	<b>15</b>	<b>60</b>

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Viva - 01 & 02	5	5	5	5	20
Skill Evaluation	3	3	3	3	12
Record	2	2	2	2	8
<b>Total</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>40</b>

### Rubric for Internal Assessment

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Punctuality and safety measures	Punctual in coming to the lab and carrying essential safety things	Less punctual and missing any safety things	Ignorant in attending practical and missing 50% safety things	Not attending and no safety things	All
Knowledge about the	Exceptional knowledge	Considerable knowledge	Minimal knowledge	Not attended	

<b>experiment</b>	<b>about experiment</b>	<b>about the experiment</b>	<b>about the experiment</b>		
<b>Handling of apparatus and recording of observation</b>	<b>Accurate handling of apparatus &amp; Accurate, precise and appropriate reporting and recording the results in SI units</b>	<b>Less proper but careful handling of apparatus &amp; Wrong but appropriate reporting and use of SI units</b>	<b>Proper but careless handling of apparatus &amp; Incorrect way of recording observation</b>	<b>Not attended</b>	
<b>Maintenance of record book</b>	<b>Perfect presentation of record in terms of completeness, neatness, well maintenance and sticking to the dead line of submission</b>	<b>Completing and fine maintenance of record. Adhering to the dead line</b>	<b>Incomplete record</b>	<b>Not submitting</b>	

**Semester III**  
**CHE1031 - Inorganic Chemistry I**

**Credit: 3**  
**Theory**

Course Outcomes		Level
CO-1	Understand various bonding theories - VB and MO theories	Understand
CO-2	Assess the reasons for existence and nonexistence of molecules	Analyze
CO-3	Explain the oxidation states of d- and f-block elements and spectral properties	Remember
CO-4	Features of co-ordination complexes and their importance in biological system	Remember

**Covalent bonding:** VB Approach: Shapes of some inorganic molecules and ions based on VSEPR and hybridization with suitable examples of linear, trigonal planar, square planar, tetrahedral, trigonal bipyramidal and octahedral arrangements. Concept of resonance and resonating structures in various inorganic and organic compounds.

**MO Approach:** Rules for the LCAO method, bonding and antibonding MOs and their characteristics for s-s, s-p and p-p combinations of atomic orbitals, nonbonding combination of orbitals, MO treatment of homonuclear diatomic molecules of 1<sup>st</sup> and 2<sup>nd</sup> periods (including idea of s-p mixing) and heteronuclear diatomic molecules such as HF, CO, NO and NO<sup>+</sup>. Polyatomic molecules BeH<sub>2</sub>, BH<sub>3</sub> and NH<sub>3</sub> - Walsh diagram. Comparison of VB and MO approaches.

**Transition Elements (3d series):** General group trends with special reference to electronic configuration, variable valency, colour, magnetic and catalytic properties, ability to form complexes and stability of various oxidation states (Latimer diagrams) for Mn, Fe and Cu.

**Lanthanoids and actinoids:** Electronic configurations, oxidation states, colour, magnetic properties, lanthanide contraction, separation of lanthanides (ion exchange method only).

**Coordination Chemistry-I:** ligands, IUPAC nomenclature – coordination number, geometries and isomerism. Theories of coordination compounds - Werner's theory

**Valence Bond Theory (VBT):** Inner and outer orbital complexes of Cr, Fe, Co, Ni and Cu (coordination numbers 4 and 6). Structural and stereoisomerism in complexes with coordination numbers 4 and 6. Drawbacks of VBT.

**Crystal Field Theory:** Crystal field effect, octahedral symmetry. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields. Tetrahedral symmetry. Factors

affecting the magnitude of  $10Dq$ . Spectrochemical series. Comparison of CFSE for  $O_h$  and  $T_d$  complexes, spectral and magnetic properties, application of CFT, Tetragonal distortion of octahedral geometry. Jahn-Teller distortion, Square planar coordination.

### Reference Books

1. B.H. Mahan, University Chemistry 3<sup>rd</sup> Ed. Narosa 1998.
2. R.H. Petrucci, General Chemistry 5<sup>th</sup> Ed. Macmillan Publishing Co., New York, 1985.
3. F.A. Cotton, & G. Wilkinson, Basic Inorganic Chemistry, Wiley.
4. D. Shriver & P. W. Atkins, Inorganic Chemistry, W. H. Freeman and Company, 5<sup>th</sup> edition, 2009.
5. G. Wulfsberg, Inorganic Chemistry, Viva Books Pvt. Ltd. 2014.
6. J.D. Lee, Concise Inorganic Chemistry, Wiley, 5<sup>th</sup> edn., 2016.
7. B.E. Douglas, D.H. McDaniel, & J.J. Alexander, Concepts and Models in Inorganic Chemistry, John Wiley & Sons. 2010.
8. J.E. Huheey, E.A. Keiter, R.L. Keiter, & O.K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education India, 2006.
9. C. N. R. Rao, Understanding Chemistry, University Press (India) Ltd., 2001.
10. R.P. Sarkar, General and Inorganic Chemistry Part- I, 3<sup>rd</sup> revised edition; New Central Book Agency, 2011.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	1	2	1	3
CO2	1	1	1	1	3
CO3	3	2	3	1	3
CO4	2	1	2	1	3

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
Total	25	25	25	25	100

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
Total	12	9	9	10	40

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)	-	5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

#### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	
Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

#### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Structuring (30 %)	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	
Drafting skill	Good	Good	< 10 %	> 10 %	

(30 %)	language &< 2 % Plagiarism	language &< 5 % Plagiarism	Plagiarism	Plagiarism	
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**MODEL QUESTION PAPER  
CHE1031 INORGANIC CHEMISTRY-I**

**PART - A                      ANSWER ALL QUESTIONS                      (10 x1 = 10marks)**

- Ni(CO)<sub>4</sub> is -----
  - Square planar and paramagnetic
  - tetrahedral and diamagnetic
  - (c) Square planar and diamagnetic
  - (d) tetrahedral and paramagnetic
- The CFSE for a low spin octahedral complex of a d<sup>7</sup> ion is ----- .
  - 2.4 Δ<sub>0</sub>
  - 1.8 Δ<sub>0</sub>
  - 1.2 Δ<sub>0</sub>
  - 0.6 Δ<sub>0</sub>

**PART - B                      ANSWER ANY FIVE QUESTIONS                      (5 x 3 = 15marks)**

- List the postulates of Werner theory.
- What is spectrochemical series ? Why is it so called ?

**Part – C**

**Answer ALL the questions                      [5 x 7M = 35 Marks]**

- What are the postulates of crystal field theory
  - What are the factors that affect the crystal field splitting energy ? How do they affect ?

[OR]

- What is inner orbital complexes ? Give some examples.
  - Explain about the Jahn teller distortion in square planar complexes.

**Semester III**  
**CHE1032 - Inorganic Chemistry Laboratory I**

**Credit: 2**

**Practical**

Course Outcomes		Level
CO-1	Quantitatively estimate the amount of metal ions from the given samples	Analyse
CO-2	Obtain expertise in preparing stock solutions and volumetric methods	Understand
CO-3	Identify cationic/anionic species with specific group separation procedures	Apply
CO-4	Develop semi-micro qualitative analytical skills	Skills

**Volumetric Analysis:**

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titrating it with  $\text{KMnO}_4$ .
3. Estimation of water of crystallization in Mohr's salt by titrating with  $\text{KMnO}_4$ .
4. Estimation of Fe (II) ions by titrating it with  $\text{K}_2\text{Cr}_2\text{O}_7$  using internal indicator.
5. Estimation of Cu (II) ions iodometrically using  $\text{Na}_2\text{S}_2\text{O}_3$ .
6. Estimation of (i)  $\text{Mg}^{2+}$  or (ii)  $\text{Zn}^{2+}$  by complexometric titrations using EDTA.
7. Estimation of total hardness of a given sample of water by complexometric titration.

**Qualitative Analysis:**

Semi-micro qualitative analysis using  $\text{H}_2\text{S}$  of mixtures - not more than four ionic species (two anions and two cations and excluding insoluble salts) out of the following:

**Cations :**  $\text{NH}_4^+$ ,  $\text{Pb}^{2+}$ ,  $\text{Ag}^+$ ,  $\text{Bi}^{3+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Sn}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Al}^{3+}$ ,  $\text{Co}^{2+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{K}^+$

**Anions :**  $\text{CO}_3^{2-}$ ,  $\text{S}^{2-}$ ,  $\text{SO}_3^{2-}$ ,  $\text{S}_2\text{O}_3^{2-}$ ,  $\text{NO}_3^-$ ,  $\text{CH}_3\text{COO}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{I}^-$ ,  $\text{NO}_2^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{PO}_4^{3-}$ ,  $\text{BO}_3^{3-}$ ,  $\text{C}_2\text{O}_4^{2-}$ ,  $\text{F}^-$  (Spot tests should be carried out wherever feasible)

**Reference Books**

1. In-house manual prepared by Department of Chemistry, CUTN, Thiruvavur.
2. G. Svehla, Vogel's Qualitative Inorganic Analysis, Pearson Education, **2012**.  
Mendham, J. Vogel's Quantitative Chemical Analysis, Pearson, **2009**.
3. G. H. Jeffery, J. Bassett, J. Mendham, and R. C. Denney, Vogel's quantitative chemical analysis, 5<sup>th</sup> edition, Longman Scientific and Technical, **1989**.

- J. Mendham, J. C. Denney, J. D. Barnesand, M. J. K.Thomas: Vogel's Prescribed book of qualitative chemical analysis, 6<sup>th</sup> Edition, Prentice Hall, **2000**.
- M. Hein, J. N. Peisen and R. L. Miner, Foundations of College Chemistry in the Laboratory, John Wiley and Sons, **2011**.
- J. D.Woollins, Inorganic experiments, 3<sup>rd</sup> Edition, Wiley-VCH Verlag GmbH Co., **2012**.
- Ghoshal, Mahapatra and Nad, An Advanced Course in Practical Chemistry, New Central Book Agency, **2011**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	1	2	1	3
CO2	1	1	1	1	3
CO3	3	2	3	1	2
CO4	2	1	2	1	3

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	15	15	15	15	60
External	10	10	10	10	40
Total	25	25	25	25	100

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Punctuality	3	3	3	3	12
Experiment skill	3	3	3	3	12
Performance in Lab	3	3	3	3	12
Maintenance of Observation Records	3	3	3	3	12
Attendance	3	3	3	3	12
Total	15	15	15	15	60

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Viva - 01 & 02	5	5	5	5	20
Skill Evaluation	3	3	3	3	12
Record	2	2	2	2	8
Total	10	10	10	10	40

### Rubric for Internal Assessment

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Punctuality and safety measures	Punctual in coming to the lab and carrying essential safety things	Less punctual and missing any safety things	Ignorant in attending practical and missing 50% safety things	Not attending and no safety things	All
Knowledge about the experiment	Exceptional knowledge about experiment	Considerable knowledge about the experiment	Minimal knowledge about the experiment	Not attended	
Handling of apparatus and recording of observation	Accurate handling of apparatus & Accurate, precise and appropriate reporting and recording the results in SI units	Less proper but careful handling of apparatus & Wrong but appropriate reporting and use of SI units	Proper but careless handling of apparatus & Incorrect way of recording observation	Not attended	
Maintenance of record book	Perfect presentation of record in terms of completeness, neatness, well maintenance and sticking to the dead line of submission	Completing and fine maintenance of record. Adhering to the dead line	Incomplete record	Not submitting	

**Semester IV**  
**CHE1041 - Organic Chemistry I**

**Credits: 3**

**Theory**

Course Outcomes		Level
CO-1	To describe the various properties of aromatic systems	Understand
CO-2	To differentiate various functional groups present in the organic compounds	Analyze
CO-3	To list the existence of various amino acids, proteins and its importance in biological processes	Remember
CO-4	To sketch classification of carbohydrates and its source in the various naturally occurring oligosaccharides	Apply

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.

**Aromatic hydrocarbons:** Preparation (case benzene) from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid. Reactions: (case benzene): Electrophilic substitution: nitration, halogenation and sulphonation. Friedel-Craft's reaction (alkylation and acylation) (upto 4 carbons on benzene). Side chain oxidation of alkyl benzenes (upto 4 carbons on benzene).

**Alkyl and Aryl Halides, Aryalkyl Halides (Upto 5 carbons):** Types of Nucleophilic Substitution ( $S_N1$ ,  $S_N2$  and  $S_Ni$ ) reactions. Preparation: from alkenes and alcohols. Reactions: hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation. Williamson's ether synthesis: Elimination vs substitution. Aryl Halides Preparation: (Chloro, bromo and iodo-benzene case): from phenol, Sandmeyer Gattermann reactions. Reactions (Chlorobenzene): Aromatic nucleophilic substitution (replacement by  $-OH$  group) and effect of nitro substituent. Benzyne Mechanism:  $KNH_2/NH_3$  (or  $NaNH_2/NH_3$ ). Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.

**Alcohols, Phenols and Ethers (Upto 5 Carbons):** Alcohols: Preparation of  $1^\circ$ ,  $2^\circ$  and  $3^\circ$  alcohols: using Grignard reagent, Ester hydrolysis, Reduction of aldehydes, ketones, carboxylic acid and esters. Reactions: With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk.  $KMnO_4$ , acidic dichromate, conc.  $HNO_3$ ). Oppeneauer oxidation Diols: (Upto 6 Carbons) oxidation of diols.

**Phenols:** Preparation: Cumenehydroperoxide method, from diazonium salts. Reactions: Electrophilic substitution: Nitration, halogenation and sulphonation. Reimer Tiemann reaction, Gattermann-Koch reaction, Houben-Hoesch Condensation, Schotten - Baumann Reaction. Ethers (aliphatic and aromatic): Cleavage of ethers with HI.

**Aldehydes and ketones (aliphatic and aromatic):** (Formaldehyde, acetaldehyde, acetone and benzaldehyde) Preparation: from acid chlorides and from nitriles. Reactions – Reaction with HCN, ROH, NaHSO<sub>3</sub>, NH<sub>2</sub>-G derivatives. Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemensen reduction and Wolff Kishner reduction. Meerwein-Ponndorf-Verley reduction.

**Carboxylic acids and their derivatives Carboxylic acids (aliphatic and aromatic):** Preparation: Acidic and Alkaline hydrolysis of esters. Reactions: Hell – Vohlard - Zelinsky Reaction. Carboxylic acid derivatives (aliphatic): (Upto 5 carbons) Preparation: Acid chlorides, Anhydrides, Esters and Amides from acids and their interconversion. Reactions: Comparative study of nucleophilicity of acyl derivatives. Reformatsky Reaction, Perkin condensation.

**Amines and Diazonium Salts Amines (Aliphatic and Aromatic) (Upto 5 carbons):** Preparation: from alkyl halides, Gabriel's Phthalimide synthesis, Hofmann Bromamide reaction. Reactions: Hofmann vs. Saytzeff elimination, Carbylamine test, Hinsberg test, with HNO<sub>2</sub>, Schotten – Baumann Reaction. Electrophilic substitution (case aniline): nitration, bromination, sulphonation. Diazonium salts: Preparation: from aromatic amines. Reactions: conversion to benzene, phenol, dyes.

**Amino Acids, Peptides and Proteins:** Preparation of Amino Acids: Strecker synthesis using Gabriel's phthalimide synthesis. Zwitterion, Isoelectric point and Electrophoresis. Reactions of Amino acids: ester of –COOH group, acetylation of –NH<sub>2</sub> group, complexation with Cu<sup>2+</sup> ions, ninhydrin test. Overview of Primary, Secondary, Tertiary and Quaternary Structure of proteins. Determination of Primary structure of Peptides by degradation Edmann degradation (N-terminal) and C-terminal (thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection (t-butyloxycarbonyl and phthaloyl) and carbon activating groups and Merrifield solid-phase synthesis.

**Carbohydrates:** Classification, and General Properties, Glucose and Fructose (open chain and cyclic structure), Determination of configuration of monosaccharides, absolute configuration of Glucose and Fructose, Mutarotation, ascending and descending in monosaccharides. Structure of disaccharides (sucrose, cellobiose, maltose, lactose) and polysaccharides (starch and cellulose) excluding their structure elucidation.

#### Reference Books

1. G.M.Barrow, Physical Chemistry, Tata McGraw-Hill, **2007**.
2. G.W. Castellan, Physical Chemistry, 4th Ed. Narosa, **2004**.
3. J.C. Kotz, P.M. Treichel & J.R.Townsend, General Chemistry, Cengage Learning India Pvt. Ltd., New Delhi, **2009**.
4. B.H. Mahan, University Chemistry, 3rd Ed. Narosa, **1998**.
5. R.H.Petrucci, General Chemistry, 5th Ed., Macmillan Publishing Co., New York **1985**.
6. I.L. Finar, Organic Chemistry, Vol I, 6th edn, Pearson Education, **2002**.
7. I.L. Finar, Organic Chemistry, Vol II, 5th edn, Pearson Education India, **2002**.
8. R.T.Morrison, R.N. Boyd, Organic Chemistry, 7th edn, Pearson Education, **2010**.
9. D. L.Nelson, M. M.Cox, Lehninger, Principles of Biochemistry, 7th edn., WH Freeman, **2017**.

10. J.M. Berg, J.L. Tymoczko, L.Stryer, Biochemistry, 5th edn, W.H.Freeman and Co Ltd, 2002.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	1	1	1	3	1
CO2	1	2	3	1	2
CO3	1	2	3	2	1
CO4	1	1	1	2	1

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
Total	25	25	25	25	100

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO 2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
Total	12	9	9	10	40

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
Total	10	14	15	21	60

**Rubric – Seminar**

<b>Criteria</b>	<b>Excellent (100 %)</b>	<b>Good (80 %)</b>	<b>Average (60 %)</b>	<b>Poor (50 %)</b>	<b>COs</b>
<b>Quality of content</b>	<b>Complete information with suitable examples</b>	<b>Complete information without suitable examples</b>	<b>Partial information with examples</b>	<b>Partial information without examples</b>	<b>All</b>
<b>Quality of Presentation</b>	<b>Perfect</b>	<b>Good</b>	<b>Average</b>	<b>Poor</b>	
<b>Q &amp; A</b>	<b>Perfect</b>	<b>Good</b>	<b>Average</b>	<b>Poor</b>	
<b>PPT skill</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>	

**Rubric – Assignment**

<b>Weightage Criteria</b>	<b>Excellent (100 %)</b>	<b>Good (80 %)</b>	<b>Average (60 %)</b>	<b>Poor (50 %)</b>	<b>COs</b>
<b>Content (40 %)</b>	<b>Complete information with suitable examples</b>	<b>Complete information without suitable examples</b>	<b>Partial information with examples</b>	<b>Partial information without examples</b>	<b>All</b>
<b>Structuring (30 %)</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>	
<b>Drafting skill (30 %)</b>	<b>Good language &amp; &lt; 2 % Plagiarism</b>	<b>Good language &amp; &lt; 5 % Plagiarism</b>	<b>&lt; 10 % Plagiarism</b>	<b>&gt; 10 % Plagiarism</b>	

**MODEL QUESTION PAPER**  
**CHE1041 Organic Chemistry**

**Duration: 3 Hours**

**Max. Marks: 60**

**Part – A**

Answer **ALL** the questions

**(10 x 1 = 10 Marks)**

1. Name and draw the structure of anti-markovnikov's product of 1-butene.
2. Predict the correct order of reactivity of alkyl halides towards  $S_N2$  reactions
  - a)  $1^\circ > 2^\circ > 3^\circ > \text{Me}$
  - b)  $\text{Me} > 1^\circ > 2^\circ > 3^\circ$
  - c)  $1^\circ > 3^\circ > \text{Me} > 2^\circ$
  - d)  $3^\circ > 2^\circ > \text{Me} > 1^\circ$

**Part – B**

Answer **ANY FIVE** questions

**(5 x 3 = 15 Marks)**

11. Write the sulphonation reaction of benzene with mechanism.
12. Explain the effect of solvent on the rate of  $S_N2$  reactions.

**Part – C**

Answer **ALL** the questions

**(5 x 7 = 35 Marks)**

18. I. a) Arrive the product for the following reaction with mechanism. (4)  
b) Write acid catalysed hydrolysis of ester with mechanism. (3)

(Or)
18. II. a) Explain the Benzyne mechanism with an example. (3)  
b) Illustrate  $S_NAr$  mechanism with an example and energy diagram. (4)
19. I. a) Tabulate the different reaction and reagents for the conversion of aldehydes and ketones to alcohols. (3)  
b) Write the iodoform reaction of aldehydes with mechanism. (4)

(Or)
19. II. a) Write the Clemmensen reduction of acetophenone with mechanism. (4)  
b) Explain the reaction of ammonia derivatives with aldehydes including general mechanism. (3)

**Semester IV**  
**CHE1042 - Organic Chemistry Laboratory I**

**Credits: 2**

**Practical**

Course Outcomes		Level
CO-1	To examine qualitative analysis <i>via</i> systematically with the functional groups present in given unknown organic compounds	Analyze
CO-2	To demonstrate preparation of stock solutions and the volumetric methods	Apply
CO-3	To describe about TLC techniques for the separation of organic compounds based on R <sub>f</sub> value	Understand
CO-4	To appraise qualitative analytical skills of the students	Evaluate

**1. Organic Qualitative Analysis:** Systematic Qualitative Analysis of Organic Compounds possessing monofunctional groups (-COOH, phenolic, aldehydic, ketonic, amide, nitro, amines) and preparation of one derivative.

**2. Preparations and characterizations:**

Separation of amino acids/organic compounds by chromatography (paper/TLC).

- a. Titration curve of glycine.
- b. Action of salivary amylase on starch and effect of temperature
- c. Differentiation between a reducing and a nonreducing sugar.

**Reference Books**

1. A.I. Vogel, A.R. Tatchell, B.S.Furnis, A.J. Hannaford & P.W.G. Smith, Text book of Practical Organic Chemistry, Prentice-Hall, 5th edition, **1996**.
2. F.G. Mann & B.C. Saunders, Practical Organic Chemistry Orient-Longman, **1960**.
3. V.K. Ahluwalia, & R. Aggarwal, Comprehensive Practical Organic Chemistry, University Press.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	1	3	2	1	3
CO2	1	3	1	1	3
CO3	2	3	2	2	3
CO4	1	3	2	1	3

## Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
<b>Internal</b>	15	15	15	15	60
<b>External</b>	10	10	10	10	40
<b>Total</b>	25	25	25	25	100

## Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Punctuality	3	3	3	3	12
Experiment skill	3	3	3	3	12
Performance in Lab	3	3	3	3	12
Maintenance of Observation Records	3	3	3	3	12
Attendance	3	3	3	3	12
<b>Total</b>	15	15	15	15	60

## Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Viva - 01 & 02	5	5	5	5	20
Skill Evaluation	3	3	3	3	12
Record	2	2	2	2	8
<b>Total</b>	10	10	10	10	40

## Rubric for Internal Assessment

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Punctuality and safety measures	Punctual in coming to the lab and carrying essential safety things	Less punctual and missing any safety things	Ignorant in attending practical and missing 50% safety things	Not attending and no safety things	All
Knowledge about the experiment	Exceptional knowledge about experiment	Considerable knowledge about the experiment	Minimal knowledge about the experiment	Not attended	
Handling of apparatus and recording	Accurate handling of apparatus &	Less proper but careful	Proper but careless	Not attended	

<b>of observation</b>	<b>Accurate, precise and appropriate reporting and recording the results in SI units</b>	<b>handling of apparatus &amp; Wrong but appropriate reporting and use of SI units</b>	<b>handling of apparatus &amp; Incorrect way of recording observation</b>		
<b>Maintenance of record book</b>	<b>Perfect presentation of record in terms of completeness, neatness, well maintenance and sticking to the dead line of submission</b>	<b>Completing and fine maintenance of record. Adhering to the dead line</b>	<b>Incomplete record</b>	<b>Not submitting</b>	

**Semester V**  
**CHE1051 - Analytical Methods in Chemistry**

**Credit: 4**

**Theory**

Course Outcomes		Level
CO-1	To attain the knowledge of spectroscopy and thermal methods	Knowledge
CO-2	To understand methodologies of separation techniques, and their essential contents, during the removal of wastages	Understand
CO-3	To develop the analytical procedures and schemes in qualitative and quantitative monitoring	Apply
CO-4	To elucidate the chemistry of molecules in different analytical environment	Skill

**Error analysis:** Errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals, Correlation & regression, correlation coefficient and linear regression.

**Optical methods of analysis:** Origin of EMR spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.

**UV-Visible Spectrometry:** Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instruments.

**Applications of UV-Visible spectroscopy:** Estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers. Woodward-Fieser Rules, Determination of composition of metal complexes using Job's method of continuous variation and mole ratio method.

**Infrared Spectrometry:** Basic principles of instrumentation (choice of source, sampling techniques, monochromator & detector) for single and double beam instruments; Factors influencing vibrational frequencies. Structural illustration through interpretation of data, Effect and importance of isotope substitution.

**Flame Atomic Absorption and Emission Spectrometry:** Basic principles of instrumentation (choice of source, monochromator, and detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples.

**Thermal methods of analysis:** Theory of thermogravimetry (TG), Differential Thermal Analysis (DTA), Differential Scanning Calorimeter (DSC) -Basic principle of instrumentation. Techniques for quantitative estimation of Ca and Mg from their mixture.

**Electroanalytical methods:** Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pKa values.

**Separation techniques:** Solvent extraction: Classification, principle and efficiency of the technique. Mechanism of extraction: extraction by solvation and chelation. Technique of extraction: batch, continuous and counter current extractions. Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media. Chromatography: Classification, principle and efficiency of the technique. Mechanism of separation: adsorption, partition & ion exchange. Development of chromatograms: frontal, elution and displacement methods. Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.

#### Reference Books

1. G.H. Jeffery, J. Bassett, J.Mendham, &R.C.Denney, Vogel's Textbook of Quantitative Chemical Analysis, 5<sup>th</sup>Ed.,John Wiley & Sons, **1989**.
2. H.H. Willard,L.L.Merritt, J.Dean, &F.A.Settoe, Instrumental Methods of Analysis, 7th Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA, **1988**.
3. G. D.Christian, Purnendu K. Dasgupta, Kevin A. Schug, Analytical Chemistry, 7<sup>th</sup> Ed., John Wiley& Sons, New York, **2004**.
4. D. C.Harris, Exploring Chemical Analysis, Ed. New York, W.H. Freeman, **2004**.
5. S.M.Khopkar, Basic Concepts of Analytical Chemistry, 3<sup>rd</sup> Ed., New Age, International Publisher, **2017**.
6. D.A.Skoog, F.J.Holler &T.A. Nieman, Principles of Instrumental Analysis, 6<sup>th</sup> Ed., Cengage Learning India Ed.**1998**.
7. O.Mikes, Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Series on Analytical Chemistry, John Wiley & Sons, **1979**.
8. R.V. Ditts, Analytical Chemistry; Methods of Separation, New York van Nostrand, **1974**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	3	1	2	1	3
CO2	2	1	2	1	3
CO3	3	2	3	1	3
CO4	2	1	3	1	3

#### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
Total	25	25	25	25	100

#### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10

<b>Seminar</b>	<b>2</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>5</b>
<b>Quiz/Test</b>	<b>5</b>	<b>5</b>	<b>5</b>	<b>5</b>	<b>20</b>
<b>Attendance</b>	<b>2</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>5</b>
<b>Total</b>	<b>12</b>	<b>9</b>	<b>9</b>	<b>10</b>	<b>40</b>

#### Mapping course outcomes with External Assessment

<b>Component</b>	<b>CO-1</b>	<b>CO-2</b>	<b>CO-3</b>	<b>CO-4</b>	<b>Total</b>
<b>Objective Qtns (10 x 1=10 Marks)</b>	<b>3</b>	<b>2</b>	<b>3</b>	<b>2</b>	<b>10</b>
<b>Descriptive (5x 3=15 Marks)</b>		<b>5</b>	<b>5</b>	<b>5</b>	<b>15</b>
<b>Long Answer Qtns (5x 7=35 Marks)</b>	<b>7</b>	<b>7</b>	<b>7</b>	<b>14</b>	<b>35</b>
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

#### Rubric – Seminar

<b>Criteria</b>	<b>Excellent (100 %)</b>	<b>Good (80 %)</b>	<b>Average (60 %)</b>	<b>Poor (50 %)</b>	<b>COs</b>
<b>Quality of content</b>	<b>Complete information with suitable examples</b>	<b>Complete information without suitable examples</b>	<b>Partial information with examples</b>	<b>Partial information without examples</b>	<b>All</b>
<b>Quality of Presentation</b>	<b>Perfect</b>	<b>Good</b>	<b>Average</b>	<b>Poor</b>	
<b>Q &amp; A</b>	<b>Perfect</b>	<b>Good</b>	<b>Average</b>	<b>Poor</b>	
<b>PPT skill</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>	

#### Rubric – Assignment

<b>Weightage Criteria</b>	<b>Excellent (100 %)</b>	<b>Good (80 %)</b>	<b>Average (60 %)</b>	<b>Poor (50 %)</b>	<b>COs</b>
<b>Content (40 %)</b>	<b>Complete information</b>	<b>Complete information</b>	<b>Partial information</b>	<b>Partial information</b>	<b>All</b>

	<b>with suitable examples</b>	<b>without suitable examples</b>	<b>with examples</b>	<b>without examples</b>	
<b>Structuring (30 %)</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>	
<b>Drafting skill (30 %)</b>	<b>Good language &amp; &lt; 2 % Plagiarism</b>	<b>Good language &amp; &lt; 5 % Plagiarism</b>	<b>&lt; 10 % Plagiarism</b>	<b>&gt; 10 % Plagiarism</b>	

**MODEL QUESTION PAPER**  
**CHE1051 Analytical Methods in Chemistry**

**Duration: 3 Hours**

**Max. Marks: 60**

**PART- A**

ANSWER ALL THE QUESTIONS

(10 x 1 = 10 MARKS)

1. Predict the energy order of different electromagnetic radiation:

- a)  $\gamma$  – rays > X – rays > Microwaves > UV light waves
- b) UV light waves > Visible light waves > Radio waves > Microwaves
- c)  $\gamma$  – rays > X – rays > Radio waves > Infrared radiation
- d) X – rays > UV light waves > Microwaves > Radio waves

2. N-H stretching vibration of amines ranges in the value of

- a) 3600 – 3500  $\text{cm}^{-1}$  b) 3500-3300  $\text{cm}^{-1}$  c) 3400 – 3500  $\text{cm}^{-1}$  d) 3400 – 3200  $\text{cm}^{-1}$

**PART B**

ANSWER ANY FIVE QUESTIONS

(5 x 3 = 15 Marks)

1. Find the suspected result and apply Q-test based on average deviation for the following data: 46.62, 46.47, 46.34, 46.53, 46.48 and 46.57.

2. How will you determine the composition of metal complexes using mole ratio method?

### PART C

ANSWER ALL THE QUESTIONS

(5 x 7 = 35 Marks)

18. (A) a) Write the significance of t-test and F-test with their formula. (3 Marks)
- b) Write about the normal distribution curve of indeterminate errors. (2 Marks)
- c) Differentiate accuracy and precision (2 Marks)

(OR)

(B). a) Discuss about the working principle of single beam UV-Vis spectrophotometer that must include about barrier cell detector with a neat sketch of its instrumentation. (4 Marks)

b) Write the fundamental laws & selection rules based on optical methods of analysis. (3 Marks)

20) (A) a) Write the sequence of steps with flow chart observed in flame atomization process.

(3 Marks)

b) Draw and explain the electrothermal atomization assembly. (4 Marks)

(OR)

(B). a) Write a short note on chromatogram. (3 Marks)

b) What are the different chromatogram development methods? (4 Marks)

## Semester V

### CHE1052- Acid-bases, Redox Reactions, s- and p- block Elements

Credit: 4

Theory

Course Outcomes		Level
CO-1	Understand the chemistry and concepts of acids and bases in different solvents	Understand
CO-2	Gain knowledge on various redox reactions and its applications	Remember
CO-3	Understand the basics of s and p block elements	Understand
CO-4	Grasp chemistry of p-block elements (B, C, N, O and halogen groups) & noble gases	Remember

**Acids and Bases, Chemistry of Aqueous and Non-aqueous Solvents:** Theory of Acid bases: Bronsted-Lowry theory, Lewis theory, Lux-Flood definition, Usanovich definition, HSAB theory and symbiosis - Gas phase acid-base chemistry – Solvent levelling effects. Chemistry in aqueous and Non-aqueous Solvents - super acids - molten salts.

**Oxidation and Reduction Reactions:** Oxidation and reduction reactions – oxidation number concept, balancing redox equations by oxidation number method and ion-electron method – equivalent weight of oxidizing and reducing agents. Disproportionation and comproportionating reaction, Redox stability in water: Frost-Ebsworth, Latimer and Pourbaix diagrams, applications of redox reactions to extraction of elements from their ores - Ellingham diagram.

**s- and p-Block Elements:** Recapitulation of s-block elements.

**Boron Group:** Introduction; oxidation states, hydrides, halides, oxides, oxo acids, hydroxides, oxoanions, nitrogen and phosphorous derivatives. Al, Ga, In and Tl salts of oxoacids and aqueous solution chemistry, organometallic compounds.

**Carbon Group:** Introduction; allotropes of carbon, Intercalation compounds of graphite; hydrides, carbides, silicides, halides, oxides, oxo acids, hydroxides; silicates; silicones, cyanogen, its derivatives and silicon nitride; aqueous solution chemistry and oxoacid salts of Sn and Pb.

**Nitrogen Group:** Introduction; oxidation states, hydrides; halides; oxides; oxo acids; salts of oxo acids; oxo anions; hydroxides; nitrides, phosphides and arsenides; Phosphazenes; aqueous solution chemistry; organic derivatives.

**Oxygen Group and Halogen Family:** Oxygen group: Introduction – Hydrides; Halides, Oxohalides and complex halides – Oxides, Oxoacids and their salts – Sulphur-nitrogen compounds – Aqueous solution chemistry of S, Se and Te – Organic derivatives.

Halogen family: comparative study of halogens and their compounds – Oxides and oxoacids of halogens (structure only) – Basic properties of halogens – Inter-halogen compounds – preparation, properties and uses – Pseudohalogens – Preparation, properties and uses of cyanogens and thiocyanogen comparison with halogens – Anomalous properties of fluorine.

**Noble gases:** Introduction – compounds of Xe, Kr and Rn – Preparation, structure and bonding – Reactivity

### Prescribed Books

1. J. E. Huheey, E. A. Keiter, R. L. Keiter and, O. K. Medhi, Inorganic Chemistry -Principles of Structure and Reactivity, 4<sup>th</sup> edition, Pearson Education, **2006**.
2. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5<sup>th</sup> edition, Oxford University Press, **2010**.
3. J.D. Lee, Concise Inorganic Chemistry, Wiley, 5<sup>th</sup> edn., **2016**.
4. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, 3<sup>rd</sup> edition, Pearson, **2004**.
5. N. N. Greenwood, and A. Earnshaw, Chemistry of the Elements, 2<sup>nd</sup> edition, Elsevier, **2005**.

### Reference Books

1. E. Stocchi, Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
2. R. M. Felder and R. W. Rousseau, Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi.
3. C. E. Housecraft and A. G. Sharpe, Inorganic Chemistry, 4<sup>th</sup> edition, Pearson, **2012**.
4. A. G. Massey, Main Group Chemistry, 2<sup>nd</sup> edition, John and Wiley & Sons, LTD, **2000**.
5. F. A. Cotton, G. Wilkinson, C. A. Murillo and, M. Bochmann, Advanced Inorganic Chemistry, 6<sup>th</sup> Edition, John Wiley & Sons, **2008**.
6. B. Douglas, D. McDaniel, and J. Alexander, Concepts and Models of Inorganic Chemistry, 3<sup>rd</sup> Edition, John Wiley & Sons, **2010**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	1	2	1	3
CO2	1	1	1	1	3
CO3	3	2	3	1	3
CO4	2	1	2	1	3

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
Total	25	25	25	25	100

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
<b>Total</b>	<b>12</b>	<b>9</b>	<b>9</b>	<b>10</b>	<b>40</b>

#### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

#### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	
Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

#### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information	Complete information	Partial information	Partial information	All

	<b>with suitable examples</b>	<b>without suitable examples</b>	<b>with examples</b>	<b>without examples</b>	
<b>Structuring (30 %)</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>	
<b>Drafting skill (30 %)</b>	<b>Good language &amp; &lt; 2 % Plagiarism</b>	<b>Good language &amp; &lt; 5 % Plagiarism</b>	<b>&lt; 10 % Plagiarism</b>	<b>&gt; 10 % Plagiarism</b>	<b>All</b>

### MODEL QUESTION PAPER

#### CHE1052- Acid-bases, Redox Reactions, s- and p- block Elements

**Duration: 3 Hours**

**Max. Marks: 60**

#### PART A

**ANSWER ALL THE QUESTIONS**

**(10 x 1 = 10 MARKS)**

- Setting of plaster of paris involves
  - oxidation with atmospheric oxygen
  - Combination with atmospheric CO<sub>2</sub>
  - Dehydration
  - Hydration to yield another hydrate
- Which of the following is used as propellant for whipping creams ?
  - N<sub>2</sub>O
  - NO
  - N<sub>2</sub>O<sub>3</sub>
  - N<sub>2</sub>O<sub>5</sub>

#### PART B

**ANSWER ANY FIVE QUESTIONS**

**(5 x 3 = 15 Marks)**

- Give three examples of freons, How are they made and how do they damage the environment.
- (i) The N-O<sup>+</sup> ion has a shorter bond length than does NO, even though the latter has extra electron. Explain.  
(ii) Why CN<sup>-</sup> is called as pseudohalogen ?

#### PART C

**ANSWER ALL THE QUESTIONS****(5 x 7 = 35 Marks)**

18. A. (i) Why hydrogen selenide is a stronger acid than hydrogen sulphide. Explain?

(ii) Which member of the following pairs is the stronger acid? Give reason based on acid-base theory (3)

(a)  $[\text{Fe}(\text{OH}_2)_6]^{3+}$  (b)  $[\text{Al}(\text{OH}_2)_6]^{3+}$  or  $[\text{Fe}(\text{OH}_2)_6]^{3+}$  or  $[\text{Ga}(\text{OH}_2)_6]^{3+}$

(c)  $\text{Si}(\text{OH})_4$  or  $\text{Ge}(\text{OH})_4$

(d)  $\text{HClO}_4$  or  $\text{HClO}$ ,

(e)  $\text{CH}_3\text{PO}_4$  or  $\text{H}_2\text{SO}_4$

(f)  $\text{H}_2\text{CrO}_4$  or  $\text{HMnO}_4$

(ii) Using Pauling's rule determine the pka of the following acid and arrange in the order of increasing strength (2)

(a)  $\text{HNO}_3$  (b)  $\text{H}_2\text{SO}_4$  (c)  $\text{HBrO}_3$  (d)  $\text{HClO}_4$

(OR)

(B) (i) Use the Drago-Wayland equation to compare the enthalpy of adduct formation for

(a)  $\text{I}_2 + (\text{C}_2\text{H}_5)_2\text{O}$  with

(b)  $\text{I}_2 + (\text{C}_2\text{H}_5)_2\text{S}$

Acids	$\text{I}_2$	Bases	$(\text{C}_2\text{H}_5)_2\text{O}$	$(\text{C}_2\text{H}_5)_2\text{S}$
EA	1.00	EB	1.08	0.57
CA	1.00	CB	3.08	6.49

ii) Which of the following oxides are acidic, basic or amphoteric in aqueous solution (3)

$\text{MgO}$ ,  $\text{SnO}$ ,  $\text{CO}_2$ ,  $\text{P}_2\text{O}_5$ ,  $\text{Sb}_2\text{O}_3$ ,  $\text{SO}_2$ ,  $\text{Al}_2\text{O}_3$ ,  $\text{BeO}$

(iii) What is HSAB theory? (2)

## CHE1053 - Organic Reaction Mechanisms and Heterocyclic Compounds

Credit: 4

Theory

Course Outcomes		Level
CO-1	To explain various properties of the nucleophilic substitution reactions	Understand
CO-2	To list various types of addition and elimination reactions	Remember
CO-3	To use the synthesis and application of carbanions	Apply
CO-4	To examine the chemistry of heterocyclic systems and its applications	Analyze

**Nucleophilic Substitution:** Structural and Solvation Effects on Reactivity: Characteristics of Nucleophilicity; Effect of Solvation on Nucleophilicity; Leaving-Group Effects ; Steric and Strain Effects on Substitution and Ionization Rates ; Effects of Conjugation on Reactivity; Neighboring-Group Participation Structure and Reactions of Carbocation Intermediates; Structure and Stability of Carbocations; Direct Observation of Carbocations; Competing Reactions of Carbocations; Mechanisms of Rearrangement of Carbocations ;Bridged (Nonclassical) Carbocations.

**Polar Addition and Elimination Reactions:**Sulfenylation and Selenenylation: Addition Reactions Involving Epoxides; Epoxides from Alkenes and Peroxidic Reagents Subsequent Transformations of Epoxides; Electrophilic Additions Involving Metal Ions; Solvomercuration Argentation—the Formation of Silver Complexes;Synthesis and Reactions of Alkylboranes Hydroboration; Reactions of Organoboranes;Enantioselective Hydroboration ;Comparison of Electrophilic Addition Reactions ;Additions to Alkynes and Allenes;Hydrohalogenation and Hydration of Alkynes ;Halogenation of Alkynes;Mercuration of Alkynes; Overview of Alkyne Additions ;Additions to Allenes.; E1, E2, E1cb and pyrolytic eliminations.

**Carbanion and other nucleophiles:** Acidity of hydrocarbons – carbanion character of organometallic compounds – carbanions stabilized by functional groups – enols, enamines and imines – carbanions as nucleophiles in  $S_N2$  reactions.

**Heterocyclic compounds:** Molecular orbital structure and aromatic characteristics of pyrrole, furan, thiophene and pyridine; Synthetic protocols and reactivity with particular focus on electrophilic substitution. Nucleophilic substitution of pyridine; comparison of basicity of pyridine, piperidine and pyrrole.

### Prescribed Books

1. F.A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edn, Springer, 2007.

- F. A. Carey, R. J. Sundberg, *Advanced Organic Chemistry, Part B: Reaction and Synthesis*, 5th edn, Springer, **2007**.

#### Reference Books

- I.L. Finar, *Organic Chemistry, Vol I*, 6th edn, Pearson Education, **2002**.
- I.L. Finar, *Organic Chemistry, Vol II*, 5th edn, Pearson Education India, **2002**.
- R. T. Morrison, R.N. Boyd, *Organic Chemistry*, 7th edn, Pearson Education, **2010**.
- S. H. Pine, *Organic Chemistry*, 5th edn, Tata McGraw Hill Education, **2006**.
- M. B. Smith, March's, *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 7th edn, Wiley, **2015**.
- J. Clayden, N. Greeves, S. Warren, *Organic Chemistry*, 2nd edn, Oxford University Press, **2014**.
- P. A. Sykes, *Guidebook to Mechanism in Organic Chemistry*, 6th edn, Pearson Education, **2003**.
- J.A. Joule, K. Mills, *Heterocyclic Chemistry*, 5th edn, Wiley-Blackwell, **2010**.
- A. R. Katritzky, C. A. Ramsden, J. A. Joule, V. V. Zhdankin, *Handbook of Heterocyclic Chemistry* 3rd edn, Elsevier, **2010**.
- R. K. Bansal, *Heterocyclic Chemistry*, 5th edn, New Age International Private Limited, **2017**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	1	2	2	1	1
CO2	1	1	2	1	1
CO3	1	2	2	1	1
CO4	1	2	3	2	2

#### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
Total	25	25	25	25	100

#### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
Total	12	9	9	10	40

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	
Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Structuring (30 %)	Perfectly ordered with suitable	Perfectly ordered without suitable	Average structuring with suitable	No order	

	schemes	schemes	examples	
<b>Drafting skill (30 %)</b>	<b>Good language &amp;&lt; 2 % Plagiarism</b>	<b>Good language &amp;&lt; 5 % Plagiarism</b>	<b>&lt; 10 % Plagiarism</b>	<b>&gt; 10 % Plagiarism</b>

## MODEL QUESTION PAPER

### CHE1053 - Organic Reaction Mechanisms and Heterocyclic Compounds

**Duration: 3 Hours**

**Max. Marks: 60**

#### PART A

**ANSWER ALL THE QUESTIONS**

**(10 x 1 = 10 MARKS)**

1. List any two nucleophiles.
2. Write the order of reactivity of halide leaving group in alkyl halides.

#### PART B

**ANSWER ANY FIVE QUESTIONS**

**(5 x 3 = 15 Marks)**

1. Write a short note on “oxymercuration reaction” and provide one example.
2. Write a short note on “Chugaev reaction”

#### PART C

**ANSWER ALL (either or) questions**

**(5 x 7 = 35 Marks)**

1(A). (i) Write a short note on “E2 stereospecific reactions”

(ii) “Menthyl chloride on dehydrochlorination gives only one product whereas neo menthyl chloride gives two products” explain.

2(A). Using an energy profile diagram explain a kinetically controlled reactions and thermodynamically controlled reactions? Illustrate the same with reference to the synthesis of enolates.

**Semester V**  
**CHE1054 - Physical States of Matter & Photochemistry**

**Credits: 4**

**Theory**

Course Outcomes		Level
CO-1	To explore and understand the basic concepts/theories in the physical states of matter & Photochemistry.	Understand
CO-2	To well-verse kinetic theory of gas molecules, critical phenomenon, molecular symmetry, light matter interaction, etc.	Understand
CO-3	To apply the basic concepts to group the molecules, to understand macro system, to develop eco-friendly refrigerator	Apply
CO-4	To create spectrophotometric tools, analytical materials, etc. of specific interest	Create

**Gaseous State:**

Postulates of Kinetic Theory of Gases and derivation of the kinetic gas equation. Maxwell Boltzmann distribution laws of molecular velocities and molecular energies (graphic representation – derivation not required) and their importance. Collision diameter, mean free path, Viscosity of gases and effect of temperature and pressure on coefficient of viscosity (qualitative treatment only).

**Real gases:** compressibility factor  $z$ , van der Waals equation of state – derivation and application in explaining real gas behaviour. Andrews isotherms of  $\text{CO}_2$ . Deviation of real gases from ideal behaviour, compressibility factor, causes of deviation. Van der Waals equation of state for real gases. van der Waals equation expressed in virial form – calculation of Boyle temperature, Isotherms of real gases, continuity of states. Critical phenomena, critical constants and their calculation from van der Waals equation. Virial. Liquefaction of gases (based on Joule-Thomson effect).

**Liquid State:**

Intermolecular forces in liquids (qualitative idea only), Structure of liquids. Unusual behavior of water. Surface tension of liquids, surface tension and temperature, interfacial tension, surface active agents, the Parachor and chemical constitution (atomic and structural parachor), Surface tension and its determination using a stalagmometer. Viscosity of a liquid and determination of coefficient of viscosity using Ostwald viscometer. Effect of temperature on surface tension and coefficient of viscosity of a liquid (qualitative treatment only).

**Liquid Crystals:**

Liquid crystals thermographic behaviour. Classification, structure of nematic and cholesteric phases. Applications of liquid crystals.

**Symmetry:**

Symmetry of molecules-symmetry elements and symmetry operations – centre of symmetry, plane of symmetry, proper and improper axes of symmetry, combination of symmetry elements,

Group multiplication table, Schoenflies symbols, Determination of point groups of simple molecules like H<sub>2</sub>O, NH<sub>3</sub> and BF<sub>3</sub>, crystallographic point groups symmetry.

#### **Solid State:**

Forms of solids. unit cells, crystal systems, Bravais lattice types and identification of lattice planes. Laws of Crystallography - Law of constancy of interfacial angles, Law of rational indices. Miller indices. X-Ray diffraction by crystals, Bragg's law. Structures of NaCl, KCl and CsCl (qualitative treatment only). Defects in crystals. Glass-Supercooled liquid.

Polymers: Introduction –Classifications – Molecular weight determination methods.

#### **Photochemistry:**

Laws of photochemistry-Grothius-Draper law, Stark-Einstein law. Jablonsky diagram qualitative description of fluorescence, phosphorescence, non-radiative processes (internal conversion, intersystem crossing). Quenching of fluorescence. Quantum yield, examples of low and high quantum yields, photochemical reactions (decomposition of HBr, isomerisation of maleic acid to fumaric acid), photosensitised reactions (photosynthesis, isomerization of 2-butene), chemiluminescence, bioluminescence.

#### **Reference books**

1. K. L. Kapoor, A Textbook of Physical chemistry, Volumes 1, Macmillan India Ltd.
2. B. R. Puri, L. R. Sharma, M. S. Pathania, Elements of Physical chemistry, Vishal Pub. Co.
3. P. Atkins and J. Paula, The elements of Physical chemistry, 7th edn., Oxford University Press.
4. D. A. McQuarrie, J. D. Simon, Physical Chemistry – A molecular Approach, Viva Books Pvt. Ltd.
5. K. J. Laidler and J. M. Meiser, Physical Chemistry 3rd Edition, Houghton Mifflin Comp., New York, International Edition, **1999**.
6. K. K. Sharma, L R Sharma, A textbook of Physical Chemistry, Vikas Publishing house.
7. I. N. Levine, Physical Chemistry, Tata Mc Graw Hill.
8. Gurdeep Raj, Photochemistry, 6th Edn, Goel Publishing House, **2014**.
9. Rohatgi-Mukherjee, Fundamentals of Photochemistry, New Age International (P) Ltd, **1978**.
10. V. Ramakrishnan and M. S. Gopinathan, Group Theory in chemistry, Vishal Publication, **1986**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	3	1	2	1	1
CO2	3	1	2	1	1
CO3	3	1	2	1	1
CO4	3	1	3	2	2

#### **Evaluation**

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
<b>Internal</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>40</b>

<b>External</b>	<b>15</b>	<b>15</b>	<b>15</b>	<b>15</b>	<b>60</b>
<b>Total</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>100</b>

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
<b>Total</b>	<b>12</b>	<b>9</b>	<b>9</b>	<b>10</b>	<b>40</b>

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	
Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Structuring (30 %)	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	
Drafting skill (30 %)	Good language & < 2 % Plagiarism	Good language & < 5 % Plagiarism	< 10 % Plagiarism	> 10 % Plagiarism	

### MODEL QUESTION PAPER

#### CHE1054 - Physical States of Matter & Photochemistry

Duration: 3 Hours

Max. Marks: 60

#### PART A

ANSWER ALL THE QUESTIONS

(10 x 1 = 10 MARKS)

1. What are F-centres?
2. What is the point group of BF<sub>3</sub>?

#### PART B

ANSWER ANY FIVE QUESTIONS

(5 x 3 = 15 Marks)

1. Explain the fluorescence and phosphorescence using Jablonski diagram.
2. What are miller indices? Sketch (222), (110) and (001) planes.

#### PART C

ANSWER ALL THE QUESTIONS

(7 x 5 = 35 Marks)

1. a) Assign various crystals into respective crystal systems & Bravais Lattice and explain their features based on axial and angular parameters.

(or)

- b) How does the rotating crystal method help us to identify the structure of NaCl?
2. a) What are photosensitized reactions? Why do the photochemical reactions prefer at T1 level? Write the chemistry of ozone formation, Hg sensitized reaction and cage effect.  
(or)
- b) Detail the kinetics of biomolecular quenching mechanism and derive the expression of Stern-Volmer equation? What is its significance?

## Semester V

### CHE1055 - Analytical & Inorganic Chemistry Laboratory I

Credit: 2

Practical

Course Outcomes		Level
CO-1	To estimate inorganic compounds from a mixture	Apply
CO-2	To value volumetric and gravimetric procedures	Evaluate
CO-3	Apply UV-Vis spectroscopy to estimate concentration of an ion in given solution	Apply
CO-4	To handle spectrophotometric tools, analytical materials, etc. of specific interest	Analyze

1. Estimation of inorganic compound in a mixture by Volumetric and Gravimetric analysis.

A mixture of solution(s) should be given for estimation

1. Cu (V) and Ni (G)
2. Fe (V) and Zn (G)
3. Fe (V) and Ni (G)
4. Zn (V) and Cu (G)

2. Draw calibration curve (absorbance at  $\lambda_{\max}$  vs. concentration) for various concentrations of a given coloured compound ( $\text{KMnO}_4/\text{CuSO}_4$ ) and estimate the concentration of the same in a given solution.

3. Determine the composition of the  $\text{Fe}^{3+}$ -salicylic acid complex solution by Job's method.

#### Reference Books

1. G. Svehla, Vogel's Qualitative Inorganic Analysis, Pearson Education, **2012**.  
Mendham, J. Vogel's Quantitative Chemical Analysis, Pearson, **2009**.
2. In-house manual prepared by Department of Chemistry, CUTN, Thiruvurur.
3. M.GhoshalandNad, An Advanced Course in Practical Chemistry, New Central Book Agency, **2011**.
4. V.Venkateswaran,R.VeeramyandA.R.Kulandaivelu, Basic principles of Practical Chemistry, 2<sup>nd</sup> edition, New Delhi, Sultan Chand & sons, **1997**.
5. M. Hein, J. N. Peisen and R. L. Miner, Foundations of College Chemistry in the Laboratory, John Wiley and Sons, **2011**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	2	2	1	3
CO2	1	2	1	1	3
CO3	2	3	3	1	3
CO4	2	3	2	1	3

## Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
<b>Internal</b>	15	15	15	15	60
<b>External</b>	10	10	10	10	40
<b>Total</b>	25	25	25	25	100

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Punctuality	3	3	3	3	12
Experiment skill	3	3	3	3	12
Performance in Lab	3	3	3	3	12
Maintenance of Observation Records	3	3	3	3	12
Attendance	3	3	3	3	12
<b>Total</b>	15	15	15	15	60

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Viva - 01 & 02	5	5	5	5	20
Skill Evaluation	3	3	3	3	12
Record	2	2	2	2	8
<b>Total</b>	10	10	10	10	40

### Rubric for Internal Assessment

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Punctuality and safety measures	Punctual in coming to the lab and carrying essential safety things	Less punctual and missing any safety things	Ignorant in attending practical and missing 50% safety things	Not attending and no safety things	All
Knowledge about the experiment	Exceptional knowledge about experiment	Considerable knowledge about the experiment	Minimal knowledge about the experiment	Not attended	
Handling of apparatus and recording	Accurate handling of apparatus &	Less proper but careful	Proper but careless	Not attended	

<b>of observation</b>	<b>Accurate, precise and appropriate reporting and recording the results in SI units</b>	<b>handling of apparatus &amp; Wrong but appropriate reporting and use of SI units</b>	<b>handling of apparatus &amp; Incorrect way of recording observation</b>		
<b>Maintenance of record book</b>	<b>Perfect presentation of record in terms of completeness, neatness, well maintenance and sticking to the dead line of submission</b>	<b>Completing and fine maintenance of record. Adhering to the dead line</b>	<b>Incomplete record</b>	<b>Not submitting</b>	

**Semester V**  
**CHE1056 - Organic Chemistry Laboratory II**

**Credit: 2**

**Practical**

Course Outcomes		Level
CO-1	To examine the elements, such as N, S, Cl, Br and I present in the unknown organic compounds.	Analyze
CO-2	To use the organic compounds separation quantitatively	Apply
CO-3	To discuss purification of organic compounds by the Column chromatography	Understand
CO-4	To perform synthesis and characterization of the organic compounds (two or three steps)	Evaluate

1. Qualitative characterization of organic compounds and detection of extra elements (N, S, Cl, Br, I) in organic compounds
2. Identification and separation of a given mixture of organic compounds by chromatography (organic compounds/amino acids such as glycine, aspartic acid, glutamic acid, tyrosine or any other amino acid).
3. Preparations, purifications of organic compounds (eg.) and discussions on mechanisms  
(a) Bromination of phenol/aniline; (b) Benzoylation of amines/phenols; (c) Oxime and 2,4-dinitrophenylhydrazone of aldehyde/ketone&(d) Diazotization of arylamines

**Reference Books**

1. A.I. Vogel, A.R.Tatchell, Furnis, B.S., A.J Hannaford,P.W.G. Smith, Textbook of Practical Organic Chemistry, Prentice-Hall, 5th edn, **1996**.
2. F.G. Mann, B.C. Saunders, Practical Organic Chemistry, 4th edn, Pearson Education India, **2009**.
3. B. D.Khosla,.V. C. Garg&A.Gulati, Senior Practical Physical Chemistry, R. Chand & Co., New Delhi, **2011**.
4. Qualitative Organic Analysis, Quantitative Organic Analysis, Pearson Education, **2011**.
5. P. B.Cranwell, L. M.Harwood, C. J. Moody, Experimental Organic Chemistry, 3rd edn, Wiley-Blackwell, **2017**.
6. V.K. Ahluwalia, R.Aggarwal, Comprehensive Practical Organic Chemistry, Universities Press, **2004**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	3	1	1	3
CO2	1	3	2	1	3

CO3	2	3	1	1	3
CO4	1	3	2	1	3

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	15	15	15	15	60
External	10	10	10	10	40
<b>Total</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>100</b>

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Punctuality	3	3	3	3	12
Experiment skill	3	3	3	3	12
Performance in Lab	3	3	3	3	12
Maintenance of Observation Records	3	3	3	3	12
Attendance	3	3	3	3	12
<b>Total</b>	<b>15</b>	<b>15</b>	<b>15</b>	<b>15</b>	<b>60</b>

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Viva - 01 & 02	5	5	5	5	20
Skill Evaluation	3	3	3	3	12
Record	2	2	2	2	8
<b>Total</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>40</b>

### Rubric for Internal Assessment

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Punctuality and safety measures	Punctual in coming to the lab and carrying essential safety things	Less punctual and missing any safety things	Ignorant in attending practical and missing 50% safety things	Not attending and no safety things	
Knowledge about the experiment	Exceptional knowledge about	Considerable knowledge about the	Minimal knowledge about	Not attended	All

	experiment	experiment	the experiment		
<b>Handling of apparatus and recording of observation</b>	Accurate handling of apparatus & Accurate, precise and appropriate reporting and recording the results in SI units	Less proper but careful handling of apparatus & Wrong but appropriate reporting and use of SI units	Proper but careless handling of apparatus & Incorrect way of recording observation	Not attended	
<b>Maintenance of record book</b>	Perfect presentation of record in terms of completeness, neatness, well maintenance and sticking to the dead line of submission	Completing and fine maintenance of record. Adhering to the dead line	Incomplete record	Not submitting	

**Semester V**  
**CHE1057 - Physical Chemistry Laboratory II**

**Credit: 2**

**Practical**

Course Outcomes		Level
CO-1	To well verse with the basic laboratory instruments	Analyze
CO-2	To present the experimental data in a scientific manner.	Evaluate
CO-3	To apply fundamental concepts and evaluate physical parameters of solutions.	Apply
CO-4	To correlate physical parameters with the chemical properties of analyte.	Remember

**Surface tension measurement (use of organic solvents excluded)**

- a) Determination of the surface tension of a liquid or a dilute solution using a stalagmometer.
- b) Study of the variation of surface tension of a detergent solution with concentration.

**Viscosity measurement (use of organic solvents excluded).**

- a) Determination of the relative and absolute viscosity of a liquid or dilute solution using an Ostwald's viscometer.
- b) Study of the variation of viscosity of an aqueous solution with concentration of solute.

**Chemical Kinetics**

- a) Initial rate method: Iodide-persulphate reaction
- b) Integrated rate method:
  - i. Acid hydrolysis of methyl acetate with hydrochloric acid.
  - ii. Saponification of ethyl acetate.
  - iii. Compare the strengths of HCl and H<sub>2</sub>SO<sub>4</sub> by studying kinetics of hydrolysis of methyl acetate

**Phase equilibria**

- a) Study of the variation of mutual solubility temperature with concentration for the phenol water system and determination of the critical solubility temperature.

Potentiometry: Potassium dichromate vs. Mohr's salt

**Conductance**

- a) Determination of cell constant
- b) Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.

**References**

1. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, **2001**.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn. McGraw Hill, **2009**.
3. B. Viswanathan, Practical Physical chemistry, Viva Pub., **2005**.

4. A.M. James, F.E. Prichard, Practical Physical Chemistry Paperback, 1974.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	3	2	2	3
CO2	2	3	2	2	3
CO3	2	2	3	2	3
CO4	2	3	3	2	3

#### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	15	15	15	15	60
External	10	10	10	10	40
Total	25	25	25	25	100

#### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Punctuality	3	3	3	3	12
Experiment skill	3	3	3	3	12
Performance in Lab	3	3	3	3	12
Maintenance of Observation Records	3	3	3	3	12
Attendance	3	3	3	3	12
Total	15	15	15	15	60

#### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Viva - 01 & 02	5	5	5	5	20
Skill Evaluation	3	3	3	3	12
Record	2	2	2	2	8
Total	10	10	10	10	40

#### Rubric for Internal Assessment

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Punctuality and safety	Punctual in coming to	Less punctual and	Ignorant in attending	Not attending	All

<b>measures</b>	<b>the lab and carrying essential safety things</b>	<b>missing any safety things</b>	<b>practical and missing 50% safety things</b>	<b>and no safety things</b>	
<b>Knowledge about the experiment</b>	<b>Exceptional knowledge about experiment</b>	<b>Considerable knowledge about the experiment</b>	<b>Minimal knowledge about the experiment</b>	<b>Not attended</b>	
<b>Handling of apparatus and recording of observation</b>	<b>Accurate handling of apparatus &amp; Accurate, precise and appropriate reporting and recording the results in SI units</b>	<b>Less proper but careful handling of apparatus &amp; Wrong but appropriate reporting and use of SI units</b>	<b>Proper but careless handling of apparatus &amp; Incorrect way of recording observation</b>	<b>Not attended</b>	
<b>Maintenance of record book</b>	<b>Perfect presentation of record in terms of completeness, neatness, well maintenance and sticking to the dead line of submission</b>	<b>Completing and fine maintenance of record. Adhering to the dead line</b>	<b>Incomplete record</b>	<b>Not submitting</b>	

## Semester VI

### CHE1061 - Nuclear, Basic Organometallic & Bioinorganic Chemistry

Credit: 4

Theory

Course Outcomes		Level
CO-1	Obtain basic knowledge in nuclear chemistry and its applications	Remember
CO-2	Understand various metallurgy principles and its applications	Understand
CO-3	Get the basics in organometallic chemistry and its applications in catalysis	Remember
CO-4	Understand the principles in bioinorganic chemistry and its role in biology	Understand

**Nuclear Chemistry I:** Introduction – composition of nucleus and nuclear forces. Nuclear stability – n/p ratio, mass defect, binding energy, packing fraction and magic numbers, shell and drop models. Isotopes – detection and separation. Isotopic constitution of elements and whole number rule. Deviation of atomic weights from whole numbers. Isobars, isotones and isomers.

**Nuclear Chemistry II:** Radioactivity – discovery, detection and measurements (Wilson cloud chamber). Radioactive emanations. Disintegration theory – modes of decay – Group displacement law – Rate of disintegration – Half life and average life – Radioactive series. Nuclear transformations – use of projectiles – nuclear reactions – fission and fusion. Nuclear reactors, radio-analytical techniques and activation analysis – neutron activation. Nuclear medicine- Single Proton Emission Tomography (SPECT) and Positron Emission Tomography (PET). Applications of nuclear science in agriculture - carbon dating - rock dating - radioactive waste disposal.

**General Principles of Metallurgy:** Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon as reducing agent. Hydrometallurgy, Methods of purification of metals (Al, Pb, Ti, Fe, Cu, Ni, Zn): electrolytic, oxidative refining, Kroll process, Parting process, van Arkel-de Boer process and Mond's process. Preparation of metals (ferrous and nonferrous) and ultrapure metals for semiconductor technology.

**Organometallic Compounds:** Definition and classification with appropriate examples based on nature of metal-carbon bond (ionic, s, p and multicentre bonds). Structures of methyl lithium, Zeise's salt and ferrocene. EAN and 16/18 rules as applied to carbonyls. Preparation, structure, bonding and properties of mononuclear and polynuclear carbonyls of 3d metals.  $\pi$ -acceptor behaviour of carbon monoxide. Synergic effects (VB approach)- (MO diagram of CO can be referred to for synergic effect to IR frequencies). Homogenous catalysis.

**Bioinorganic Chemistry-I: General Principles of Bioinorganic Chemistry:** A brief introduction to bioinorganic chemistry-occurrence and availability of Inorganic elements in biological systems. Basics of Biomineralization.Uptake, transport and storage of metal ions by organisms - structure and functions of biological membranes – the generation of concentration gradients (the  $\text{Na}^+$  - $\text{K}^+$  pump); Role of  $\text{Mg}^{2+}$  ions in energy production and chlorophyll. Biologically important coordination compounds - haemoglobin, myoglobin, carbonic anhydrase and vitamin  $\text{B}_{12}$  - Their structure and application. Role of  $\text{Ca}^{2+}$  in blood clotting, stabilization of protein structures and structural role (bones).

### Prescribed Books

1. J. E.Huheey, E. A.Keiter, R. L. Keiter, and O. K.Medhi, Inorganic Chemistry - Principles of Structure and Reactivity, 4<sup>th</sup> edition, Pearson Education, **2006**.
2. P.Atkins, T.Overton, J. Rourke, M.Weller and F.Armstrong, Inorganic Chemistry, 5<sup>th</sup>edition, Oxford University Press, **2010**.
3. J. D.Lee, Concise Inorganic Chemistry, 5<sup>th</sup> edition, Wiley, **2016**.
4. S. J. Lippard and J. M.Berg, Principles of Bioinorganic Chemistry, Panima Publishing Company, New Delhi, **1997**.
5. W.Kaim and B.Schewederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, New York, USA, **2013**.
6. H. J.Arnika, Essentials of Nuclear Chemistry, 4<sup>th</sup> edition, New Age International Publishers Ltd., New Delhi, **1995**.
7. W. D.Loveland, D. J.Morrissey and G. T.Seaborg, Modern Nuclear Chemistry, Wiley-VCH Verlag GmbH Co. KGaA, **2006**.
8. Glasstone, Source Book on Atomic Energy, 3<sup>rd</sup> edition, Affiliated East West Press, **1979**.
9. B. D. Gupta and A.J. Elias, Basic Organometallic Chemistry: Concepts, Syntheses, and Applications of Transition Metals, 1<sup>st</sup> edition, Universities Press, CRC Press, **2010**.
10. R. H.Crabtree, Organometallic Chemistry of the Transition Metals, Wiley, New York, **1988**.
11. C. E.Housecraft and A.G. Sharpe, Inorganic Chemistry, 4<sup>th</sup>edition, Pearson, **2012**.

### Reference Books

1. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, 3rd edition, Pearson, **2004**.
2. G. Chatwal and M.S.Yadu, 'Coordination Chemistry', 1st edition, Himalaya Publishing House, **1992**.
3. B.Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd edition, John Wiley & Sons, **2010**.
4. F. A.Cotton, G.Wilkinson, C. A. Murillo and M.Bochmann, Advanced Inorganic Chemistry, 6th edition, John Wiley & Sons, **2008**.
5. M. C.Day Jr, and J. Selbin, Theoretical Inorganic Chemistry, Literary Licensing, LLC, **2012**.
6. H. E.Boyer, and T. L.Gall, Metals Handbook, Desk edition, **1984**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5

<b>CO1</b>	2	1	2	3	3
<b>CO2</b>	1	1	1	3	3
<b>CO3</b>	3	2	3	3	3
<b>CO4</b>	2	1	2	2	3

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
<b>Internal</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>40</b>
<b>External</b>	<b>15</b>	<b>15</b>	<b>15</b>	<b>15</b>	<b>60</b>
<b>Total</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>100</b>

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
<b>Assignment</b>	<b>3</b>	<b>2</b>	<b>2</b>	<b>3</b>	<b>10</b>
<b>Seminar</b>	<b>2</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>5</b>
<b>Quiz/Test</b>	<b>5</b>	<b>5</b>	<b>5</b>	<b>5</b>	<b>20</b>
<b>Attendance</b>	<b>2</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>5</b>
<b>Total</b>	<b>12</b>	<b>9</b>	<b>9</b>	<b>10</b>	<b>40</b>

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
<b>Objective Qtns (10 x 1=10 Marks)</b>	<b>3</b>	<b>2</b>	<b>3</b>	<b>2</b>	<b>10</b>
<b>Descriptive (5x 3=15 Marks)</b>		<b>5</b>	<b>5</b>	<b>5</b>	<b>15</b>
<b>Long Answer Qtns (5x 7=35 Marks)</b>	<b>7</b>	<b>7</b>	<b>7</b>	<b>14</b>	<b>35</b>
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
<b>Quality of content</b>	<b>Complete information with suitable examples</b>	<b>Complete information without suitable examples</b>	<b>Partial information with examples</b>	<b>Partial information without examples</b>	<b>All</b>

<b>Quality of Presentation</b>	<b>Perfect</b>	<b>Good</b>	<b>Average</b>	<b>Poor</b>	
<b>Q &amp; A</b>	<b>Perfect</b>	<b>Good</b>	<b>Average</b>	<b>Poor</b>	
<b>PPT skill</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>	

**Rubric – Assignment**

<b>Weightage Criteria</b>	<b>Excellent (100 %)</b>	<b>Good (80 %)</b>	<b>Average (60 %)</b>	<b>Poor (50 %)</b>	<b>COs</b>
<b>Content (40 %)</b>	<b>Complete information with suitable examples</b>	<b>Complete information without suitable examples</b>	<b>Partial information with examples</b>	<b>Partial information without examples</b>	<b>All</b>
<b>Structuring (30 %)</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>	
<b>Drafting skill (30 %)</b>	<b>Good language &amp; &lt; 2 % Plagiarism</b>	<b>Good language &amp; &lt; 5 % Plagiarism</b>	<b>&lt; 10 % Plagiarism</b>	<b>&gt; 10 % Plagiarism</b>	

**MODEL QUESTION PAPER**

**CHE1061 - Nuclear, Basic Organometallic & Bioinorganic Chemistry**

**Duration: 3 Hours**

**Max. Marks: 60**

**Part – A**

**Answer ALL the questions**

**(10 x 1 = 10 Marks)**

1. What is the role of manganese ion in photosystem II?
2. After oxygen molecules bind with deoxy-hemoglobin, the spin state of iron in oxy haemoglobin is converted from low spin to high spin. True/false

**Part – B**

Answer ANY FIVE questions

(5 x 3 = 15 Marks)

1. Define the following term. (a) Compartmentalisation (b) endocytosis (c) theranostic agents
2. How does  $\text{Ca}^{2+}$  -ATPase maintain the low cytosolic calcium levels in the muscle cells?  
Explain with the help of diagram.

**Part – C**

Answer ANY FIVE questions

(5 x 7 = 35 Marks)

1. (a) Identify the suitable metal (1st row transition metal) based on 18 electron rule. (4)  
(i)  $(\eta^5\text{-C}_5\text{H}_5)\text{M}(\text{CO})_2\text{Cl}$  (ii)  $[(\eta^5\text{-C}_5\text{H}_5)_2\text{M}]^+$  (iii)  $[(\eta^5\text{-C}_5\text{H}_5)\text{M}(\text{CO})_3]_2$  (iv)  $\text{HM}(\text{CO})_5$   
(b) For the given compounds, calculate a) the total number of M-M bonds in each molecule and  
b) the number of M-M bonds each metal makes with the other metal. Also draw the most appropriate structure in each case. (3)  
(i)  $\text{Os}_3(\text{CO})_{12}$  (ii)  $[(\eta^5\text{-C}_5\text{H}_5)_2\text{Fe}_2(-\text{CO})_3]$  (iii)  $[\text{Ru}_3(\text{CO})_{10}(\text{PPh}_3)_2]$

19. (a) Match the following Column A with Column B (3)

Column A

Column B

- (i) Calmodulin -
- (ii) Troponin C -
- (iii) Vitamin B12 -
- (iv) Peroxisomes -
- (v) Valinomycin -
- (vi) Amyloids -

A pool of answers for Column B:  $\text{Ca}^{2+}$  -dependent intracellular regulatory protein, Liver cells, Muscle contraction, Removal of harmful hydrogen peroxide, Phagocytosis, Alzheimer's disease, Vitamin D dependent uptake of  $\text{Ca}^{2+}$ , An ionophore

- (b) Fill in the blanks (4)

- (i) ..... ring present in chlorophyll a.
- (ii) ..... ring present in Vitamin B12.
- (iii) ..... enzyme involved in the synthesis of protoporphyrin IX
- (iv)..... is an anticoagulant of blood.

## Semester VI

### CHE1062 -Reaction Mechanisms & Natural Products Chemistry

Credit: 4

Theory

Course Outcomes		Level
CO-1	To describe basic knowledge in the organic transformations based on carbanion	Understand
CO-2	To examine the classification of organic reactions and rearrangement reactions	Analyze
CO-3	To state functions of alkaloids and the terpenoids compounds	Remember
CO-4	To sketch the importance of vitamins in biological systems	Apply

**Organic transformations based on carbanions:** Dicarboxylic acids, dicarbonyls, diesters, Acidity of  $\alpha$ -hydrogens, alkylation of diethyl malonate and ethyl acetoacetate. Synthesis using diethyl malonate and ethyl acetoacetate, Claisen condensation. Knoevenagel condensation, Dieckmann condensation.

**Molecular rearrangements:** classification – electrophilic, nucleophilic and free radical rearrangements, mechanisms of the following rearrangements: pinacol-pinacolone, Wagner – Meerwin, Tiffenev-Demjanov, Hofmann, Schmidt, Lossen, Curtius, Beckmann, Fries, Baeyer – Villager, Stevens and Benzil – Benzilic Acid Rearrangement.

#### Natural products, biomolecules and biosynthesis:

Occurrence, importance, classification and structural elucidations of natural products and biomolecules. Alkaloids: Synthesis of nicotine and piperine, morphine, cocaine. Terpenes: - Isoprene rule, structure and synthesis of citral, geraniol and  $\alpha$ -terpineol. Vitamins: Chemical constitution and physiological functions of vitamins A (Retinol) B2 (Riboflavin), vitamin C (Ascorbic acid) Natural pigments: Flavones, flavanones, isoflavones, xanthenes, quinones, pterins, chlorophyll and haemin.

#### Prescribed Books

1. F.A.Carey, R.J. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edn, Springer, 2007.
2. F.A.Carey, R.J. Sundberg, Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th edn, Springer, 2007.
3. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th edn, Wiley, 2015.
4. R.H.Thomson, The Chemistry of Natural Products, 2nd edn, Springer, 1993.

## Reference Books

1. I.L Finar, Organic Chemistry, Vol I, 6th edn, Pearson Education, **2002**.
2. I.L Finar, Organic Chemistry, Vol II, 5th edn, Pearson Education India, **2002**.
3. R.T.Morrison, Boyd, R.N. Organic Chemistry, 7th edn, Pearson Education, **2010**.
4. S. H. Pine, Organic Chemistry, 5th edn, Tata McGraw Hill Education, **2006**.
5. M. B Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th edn, Wiley, **2015**.
6. W.Carruthers,I.Coldham, Modern Methods of Organic Synthesis, 4th edn, Cambridge University Press, **2015**.
7. J.Clayden,N.Greeves,S.Warren, Organic Chemistry,2<sup>nd</sup>edn.,Oxford University Press, **2014**.
8. P. A Sykes, Guidebook to Mechanism in Organic Chemistry, 6th edn, Pearson Education, **2003**.
9. D. L.Nelson, Cox, M. M. Lehninger's Principles of Biochemistry, 7th edn., WH Freeman, **2017**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	1	1	2	1	1
CO2	1	3	2	1	1
CO3	2	2	2	3	1
CO4	1	2	2	1	3

## Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
Total	25	25	25	25	100

## Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
Total	12	9	9	10	40

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	
Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All

<b>Structuring (30 %)</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>	<b>All</b>
<b>Drafting skill (30 %)</b>	<b>Good language &amp;&lt; 2 % Plagiarism</b>	<b>Good language &amp;&lt; 5 % Plagiarism</b>	<b>&lt; 10 % Plagiarism</b>	<b>&gt; 10 % Plagiarism</b>	

### MODEL QUESTION PAPER

#### CHE1062 -Reaction Mechanisms & Natural Products Chemistry

**Duration: 3 Hours**

**Max. Marks: 60**

#### Part – A

Answer ALL the questions

(10 x 1 = 10 Marks)

- Write the structure of 1-phenylbutan-2-one
- Tollen test is positive for
  - Esters
  - Carbohydrates
  - Aldehydes
  - Ketones

#### Part – B

Answer ANY FIVE questions

(5 x 3 = 15 Marks)

- Write about Mukhaiyama aldol reaction.
- Give a synthetic protocol for  $\beta$ -ketoester preparation .

#### Part – C

Answer either or questions

(5 x 7 = 35 Marks)

1(A) (i) Explain how citral is different from geraniol. Write any one method of synthesis of geraniol. (6 Marks)

(ii) Draw the structure of ascorbic acid. (1Mark)

(or)

1(B) (i) Write a short note on Baker Venkatraman synthesis of flavanols.(4 Marks)

(ii) Draw the structure of following flavanoids. (3 Marks)

- Flavone
- Isoflavone
- Chalcone

## Semester VI

### CHE1063 - Quantum Chemistry & Molecular Spectroscopy

Credit: 4

#### Theory

Course Outcomes		Level
CO-1	To examine the meaning of wave function, its application in molecular modelling and fundamentals of spectroscopy	Analyze
CO-2	To evaluate molecular physical phenomena as a function of spectral parameters	Evaluate
CO-3	To apply the postulates of quantum mechanics in model systems.	Apply
CO-4	To understand the spectroscopic techniques	Understand

#### Quantum Chemistry I:

Classical mechanics –disadvantages. Introduction to Quantum mechanical ideas: Black body radiation, Photoelectric effect, Compton Effect, Heisenberg uncertainty principle. **Elements of Quantum mechanics:** Postulates of quantum mechanics, wave functions, quantum mechanical operators and observables, Schrödinger equation.

**Application of Schrodinger equation:** Particle-in-a-box(1D, 2D and 3D boxes), Quantum Mechanical tunnelling, Simple harmonic oscillator, Particle in a ring.

Rigid rotator - model of rotation of diatomic molecule. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution. Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, and quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus.

#### Molecular Spectroscopy I:

Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation.

**Rotation spectroscopy:** Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

**Vibrational spectroscopy:** Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Fingerprint region, Fermi resonance.

**Raman spectroscopy:** Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

**Electronic spectroscopy:** Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model.

**Nuclear Magnetic Resonance (NMR) spectroscopy:** Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales, spin-spin coupling and high resolution spectra.

**Electron Spin Resonance (ESR) spectroscopy:** Its principle, hyperfine structure, ESR of simple radicals.

### Reference Books

1. R.K. Prasad, Quantum Chemistry, New Age International, **2001**.
2. J. P. Lowe & K. Peterson, Quantum Chemistry, 3<sup>rd</sup> Ed., Academic Press, **2006**.
3. Mc Quarrie, J. D. Simon, Physical Chemistry – A molecular Approach, Viva Books.
4. I.N. Levine, Physical Chemistry, 7<sup>th</sup> Ed., Tata McGraw Hill, **2016**.
5. Gurdeep Raj, Advanced Physical Chemistry, Goel Publishing House
6. C. N. Banwell, & E. M. Mc Cash, Fundamentals of Molecular Spectroscopy, 4th Ed. Tata McGraw-Hill, New Delhi, **2006**.
7. Manas Chanda, Atomic structure and Chemical bonding in Molecular Spectroscopy, Tata McGraw Hill.
8. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to spectroscopy, 3rd edn, Thomson Brooks/Cole, **2001**.
9. D. N. Satyanarayana, Electronic absorption spectroscopy and related techniques, Universities Press.
10. D.N. Sathyanarayana, Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR, IK International, **2009**.
11. Puri, Sharma & Pathania, Principles of Physical Chemistry, Vishal Publishing Co.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	1	3	3	1
CO2	2	1	3	3	1
CO3	2	1	2	3	1
CO4	2	2	3	3	1

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
Total	25	25	25	25	100

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5

Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
<b>Total</b>	<b>12</b>	<b>9</b>	<b>9</b>	<b>10</b>	<b>40</b>

#### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

#### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	
Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

#### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information with	Complete information without	Partial information with	Partial information without	All

	suitable examples	suitable examples	examples	examples	
<b>Structuring (30 %)</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>	<b>All</b>
<b>Drafting skill (30 %)</b>	<b>Good language &amp; &lt; 2 % Plagiarism</b>	<b>Good language &amp; &lt; 5 % Plagiarism</b>	<b>&lt; 10 % Plagiarism</b>	<b>&gt; 10 % Plagiarism</b>	

### MODEL QUESTION PAPER

#### CHE1063 - Quantum Chemistry & Molecular Spectroscopy

**Duration: 3 Hours**

**Max. Marks: 60**

**Answer ALL the questions**

**(10 x 1 = 10 marks)**

1. The first emission line in the atomic spectrum of hydrogen in the Balmer series appears at

- a.  $5R/36 \text{ cm}^{-1}$       b.  $3R/4 \text{ cm}^{-1}$       c.  $7R/144 \text{ cm}^{-1}$       d.  $9R/400 \text{ cm}^{-1}$

2. The first Bohr orbit of hydrogen atom ( $n=1$ ) has  $-13.6 \text{ eV}$  energy. The possible energy value of the first excited state ( $n=2$ ) for electron is

- a.  $-54.4 \text{ eV}$       b.  $-13.6 \text{ eV}$       c.  $-3.4 \text{ eV}$       d.  $-2.4 \text{ eV}$

#### Part B

**Answer any FIVE questions**

**(5 x 3 = 15 marks)**

- Give any two postulates of quantum mechanics.
- Write a short note on Photo electric effect.

#### Part C

**Answer ALL the questions**

**(5 x 7 = 35 marks)**

- A) i) Discuss the solution of the Schrödinger wave equation for a particle in one-dimensional box. (5)

ii) Calculate the energy levels  $E_1$  to  $E_6$  for an electron in a one-dimensional box of length  $12 \times 10^{-10}$  m. How large is the energy difference between  $E_6 - E_5$  in  $\text{cm}^{-1}$ . (2)

**(OR)**

B) i) Solve the Schrodinger wave equation for a simple harmonic oscillator and solve for its energy eigen values. (5)

ii) A particle of mass  $m = 1.0 \times 10^{-26}$  g is confined to move in a box of length  $2.0 \times 10^{-10}$  m.

What is the probability of finding the particle between  $1.6 \times 10^{-10}$  m and  $1.6001 \times 10^{-10}$  m.

Calculate for  $n = 1$  and  $n = 2$ . (2)

2. A) i) Derive an expression for the energy of a rigid rotor using Schrödinger wave equation.

(5)

ii) Write a short note on average and most probable distances

of an electron from the nucleus. (2)

**(OR)**

i) Explain Spherical harmonics and discuss its solution.(5)

ii) Calculate the Spherical harmonics  $Y_{1,1}$  and  $Y_{2,0}$  (2)

## Semester VI

### CHE1064 -Analytical & Inorganic Chemistry Laboratory II

Credit: 2

#### Practical

Course Outcomes		Level
CO-1	Understand the important aspects of HSAB principles for separation and identification of inorganic ions	Understand
CO-2	Use systematic semi-micro qualitative technique for identifying rare cations	Apply
CO-3	Use semi-micro qualitative technique for separation of alkaline earth metals	Apply
CO-4	Examine the qualitatively for the transition metal ions in different oxidation states	Skills

Semi-micro qualitative analysis of a mixture containing two common and two rare - cations.

#### Reference Books:

1. G.Svehla, Vogel's Qualitative Inorganic Analysis, Pearson Education, **2012**.
2. J.Mendham, Vogel's Quantitative Chemical Analysis, Pearson, **2009**.
3. Ghoshal, Mahapatra and Nad, An Advanced Course in Practical Chemistry, New Central Book Agency, **2011**.
4. V.Venkateswaran,R.Veerassamy A.R Kulandaivelu, Basic principles of Practical Chemistry, 2nd edition, New Delhi, Sultan Chand & sons, **2016**.

#### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	15	15	15	15	60
External	10	10	10	10	40
Total	25	25	25	25	100

#### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Punctuality	3	3	3	3	12
Experiment skill	3	3	3	3	12

Performance in Lab	3	3	3	3	12
Maintenance of Observation Records	3	3	3	3	12
Attendance	3	3	3	3	12
<b>Total</b>	<b>15</b>	<b>15</b>	<b>15</b>	<b>15</b>	<b>60</b>

#### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Viva - 01 & 02	5	5	5	5	20
Skill Evaluation	3	3	3	3	12
Record	2	2	2	2	8
<b>Total</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>40</b>

#### Rubric for Internal Assessment

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Punctuality and safety measures	Punctual in coming to the lab and carrying essential safety things	Less punctual and missing any safety things	Ignorant in attending practical and missing 50% safety things	Not attending and no safety things	All
Knowledge about the experiment	Exceptional knowledge about experiment	Considerable knowledge about the experiment	Minimal knowledge about the experiment	Not attended	
Handling of apparatus and recording of observation	Accurate handling of apparatus & Accurate, precise and appropriate reporting and recording the results in SI units	Less proper but careful handling of apparatus & Wrong but appropriate reporting and use of SI units	Proper but careless handling of apparatus & Incorrect way of recording observation	Not attended	
Maintenance of record book	Perfect presentation of record in terms of completeness, neatness, well maintenance and	Completing and fine maintenance of record. Adhering to the dead line	Incomplete record	Not submitting	

sticking to  
the dead  
line of  
submission

Semester VI

CHE1065 -Organic Chemistry Laboratory III

Credit 2

Practical

Course Outcomes		Level
CO-1	To organize organic preparations based on the various one or two step reactions	Analyze
CO-2	To predict synthetic aspects of organic reactions involving the rearrangement and photochemical reactions.	Apply
CO-3	To discuss isolation of natural products by the various isolation methods	Understand
CO-4	To test the characterization of different natural products such as Caffeine, Casein, piperine and lycopene by using various analytical and spectroscopic-methods.	Evaluate

1. Preparations: Two-step preparations (any three) involving acetylation, methylation, condensation, rearrangements and photochemical reactions.

2. Isolation and characterization of natural products:

- Isolation of caffeine from tea dust
- Isolation of casein from milk
- Isolation of piperine from pepper
- Isolation of lycopene from tomato

Reference Books

- A.I. Vogel, A.R. Tatchell, B.S. Furnis, A.J. Hannaford, P.W.G. Smith, Textbook of Practical Organic Chemistry, Prentice-Hall, 5th edn, 1996.
- F.G. Mann, B.C. Saunders, Practical Organic Chemistry, 4th edn, Pearson Education India, 2009.
- B. D. Khosla, V. C. Garg & A. Gulati, Senior Practical Physical Chemistry, R. Chand & Co., New Delhi, 2011.
- B.J. Leonard, G. Lygo, Procter, Advanced Practical Organic Chemistry, 3rd edn, CRC Press, 2013.
- V.K. Ahluwalia, R. Aggarwal, Comprehensive Practical Organic Chemistry, Universities Press, 2004.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	1	3	2	2	3
CO2	1	3	2	1	3
CO3	1	3	2	1	3
CO4	2	3	1	2	3

Evaluation

Course Outcomes	
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	CO-1	CO-2	CO-3	CO-4	Total
<b>Internal</b>	15	15	15	15	60
<b>External</b>	10	10	10	10	40
<b>Total</b>	25	25	25	25	100

#### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Punctuality	3	3	3	3	12
Experiment skill	3	3	3	3	12
Performance in Lab	3	3	3	3	12
Maintenance of Observation Records	3	3	3	3	12
Attendance	3	3	3	3	12
<b>Total</b>	15	15	15	15	60

#### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Viva - 01 & 02	5	5	5	5	20
Skill Evaluation	3	3	3	3	12
Record	2	2	2	2	8
<b>Total</b>	10	10	10	10	40

#### Rubric for Internal Assessment

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Punctuality and safety measures	Punctual in coming to the lab and carrying essential safety things	Less punctual and missing any safety things	Ignorant in attending practical and missing 50% safety things	Not attending and no safety things	All
Knowledge about the experiment	Exceptional knowledge about experiment	Considerable knowledge about the experiment	Minimal knowledge about the experiment	Not attended	
Handling of apparatus and recording of observation	Accurate handling of apparatus & Accurate, precise and appropriate	Less proper but careful handling of apparatus & Wrong but	Proper but careless handling of apparatus &	Not attended	

	<b>reporting and recording the results in SI units</b>	<b>appropriate reporting and use of SI units</b>	<b>Incorrect way of recording observation</b>		
<b>Maintenance of record book</b>	<b>Perfect presentation of record in terms of completeness, neatness, well maintenance and sticking to the dead line of submission</b>	<b>Completing and fine maintenance of record. Adhering to the dead line</b>	<b>Incomplete record</b>	<b>Not submitting</b>	

**Semester VI**  
**CHE1066 - Physical Chemistry Laboratory III**

**Credit: 2**

**Practical**

Course Outcomes		Level
CO-1	To recognize various QM software and spectroscopic (UV-VIS) methods	Understand
CO-2	To perform geometry optimization and spectroscopic experiments	Analyze
CO-3	To predict the energy gap, dipole moments and stability of organic molecules	Apply
CO-4	To evaluate and study the energy, concentration, structures and kinetics using various spectroscopic methods	Evaluate

**Quantum Mechanics:**

1. Optimization of Geometry and single point energy calculations of Organic molecules
2. Calculation of energy gap between HOMO and LUMO in simple molecules and visualization of molecular orbitals
3. Calculation of dipole moment in polar organic molecules.
4. Prediction of the stability of ortho, meta, para products of nitration of aromatic ring using computational chemistry calculations.
5. Calculation of IR stretching frequencies of groups and visualization of normal modes of vibration in organic molecules.

**Spectroscopy:**

1. Study the 200-500 nm absorbance spectra of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  (in 0.1 M  $\text{H}_2\text{SO}_4$ ) and determine the  $\lambda_{\text{max}}$  values. Calculate the energies of the two transitions in different units ( $\text{J molecule}^{-1}$ ,  $\text{kJ mol}^{-1}$ ,  $\text{cm}^{-1}$ , eV).
2. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of  $\text{K}_2\text{Cr}_2\text{O}_7$ .
3. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.
4. Verify Lambert-Beer's law and determine the concentration of  $\text{CuSO}_4/\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$  in a solution of unknown concentration
5. Determine the concentrations of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  in a mixture.
6. Study the kinetics of iodination of propanone in acidic medium.
7. Determine the amount of iron present in a sample using 1,10-phenanthroline.
8. Determine the dissociation constant of an indicator (phenolphthalein).
9. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.

10. Analyse the given vibration-rotation spectrum of HCl(g)

#### Reference Books

1. J. Foresman & A. Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 2000.
2. D.C. Young, Computational Chemistry, A Practical Guide for Applying Techniques to Real World Problems, John Wiley & Sons, 2001.
3. D. Rogers, Computational Chemistry Using the PC, 3rd Edition, John Wiley & Sons, 2003.
4. A. Leach, Molecular Modelling, Principles and Applications, 2nd Edn, Longman, 2001.
5. J. M. Haile, Molecular Dynamics Simulation: Elementary Methods 2001.
6. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
7. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn. McGraw Hill, 2009.
8. Saroj Kumar and Naba Kumar, Physical Chemistry Practical, New Central Book Agency, 2012.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	1	3	2	3	3
CO2	1	3	2	3	3
CO3	1	3	2	3	3
CO4	1	3	2	3	3

#### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	15	15	15	15	60
External	10	10	10	10	40
Total	25	25	25	25	100

#### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Punctuality	3	3	3	3	12
Experiment skill	3	3	3	3	12
Performance in Lab	3	3	3	3	12
Maintenance of Observation Records	3	3	3	3	12
Attendance	3	3	3	3	12
Total	15	15	15	15	60

#### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Viva - 01 & 02	5	5	5	5	20
Skill Evaluation	3	3	3	3	12
Record	2	2	2	2	8
<b>Total</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>40</b>

#### Rubric for Internal Assessment

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Punctuality and safety measures	Punctual in coming to the lab and carrying essential safety things	Less punctual and missing any safety things	Ignorant in attending practical and missing 50% safety things	Not attending and no safety things	All
Knowledge about the experiment	Exceptional knowledge about experiment	Considerable knowledge about the experiment	Minimal knowledge about the experiment	Not attended	
Handling of apparatus and recording of observation	Accurate handling of apparatus & Accurate, precise and appropriate reporting and recording the results in SI units	Less proper but careful handling of apparatus & Wrong but appropriate reporting and use of SI units	Proper but careless handling of apparatus & Incorrect way of recording observation	Not attended	
Maintenance of record book	Perfect presentation of record in terms of completeness, neatness, well maintenance and sticking to the dead line of submission	Completing and fine maintenance of record. Adhering to the dead line	Incomplete record	Not submitting	

**Semester VII**  
**CHE1071- Solid State, Main Group & Coordination Chemistry**

**Credit: 4**

**Theory**

Course Outcomes		Level
CO-1	<b>Gain knowledge in solid state chemistry and its applications</b>	<b>Knowledge</b>
CO-2	<b>Understand the chemistry of main group elements - rings, chains and clusters</b>	<b>Understand</b>
CO-3	<b>Grasp the basic principles and their application in coordination chemistry</b>	<b>Apply</b>
CO-4	<b>Understand the principles of inorganic reaction mechanisms</b>	<b>Skills</b>

**Synthesis and modification of inorganic solids:** Structures of ionic crystals – AX and AX<sub>2</sub> type crystal structures – layer structures - lattice energy - Born-Landé, Born-Mayer and Kapustinskii equations – Derivations and applications –Review of defects in ionic solids - Thermodynamic effects of defects. Band theory, n- and p- type semiconductors and superconductors. Reactions in solid state - diffusion, diffusion coefficient, diffusion mechanisms, vacancy and interstitial diffusion, thermal decomposition of solids -Type I and Type II reactions. Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods. Hydrides and hydrogen storage materials – Inorganic pigments. Molecular material and fullerides, molecular materials & chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystals.

**The Chemistry of the Main Group Elements:** Inorganic Rings, chains, and cages Catenation and Heterocatenation, Heterocyclic ring system- Borazines, Phosphazines- Monomer and Polymer, S-N ring compounds, Homocyclic rings of S, Se and Te. Silicate minerals, Isopolyanions, Boranes: boron cage compounds-closo, nido, arachno, carboranes; cage compounds of S and P. Metal cluster: metal-metal bonding and reactivity of di-, tri- and polynuclear clusters.

**Coordination Chemistry II:** Recapitulation of Crystal field theory - splitting of d-orbitals under various geometries - Limitations of CFT – Ligand field Theory - MO theory – sigma – and pi-bonding in complexes and evidences for  $\pi$ -bonding – nephelauxetic effect – angular overlap model. Studies of coordination compounds in solution – detection of complex formation in solution – Stability constants – stepwise and overall formation constants – simple methods (Potentiometric, pH metric and photometric methods) of determining the formation constants - factors affecting stability – Irving-William series -statistical and chelate effects – forced configurations.

**Coordination Chemistry-III:** 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 – complementary and non-complementary types – inner sphere and outer sphere processes – Excited state outer sphere electron transfer reactions - isomerisation and racemisation reactions of complexes – reactions of four and six-coordinate complexes – interconversion between stereoisomers.

#### Prescribed Books

1. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, Inorganic Chemistry - Principles of Structure and Reactivity, 4th edition, Pearson Education, **2006**.
2. P. W. Atkins and J. Paula, Physical Chemistry, Oxford Publications, 8<sup>th</sup> edition, **2009**.
3. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd edition, John Wiley & Sons, **2010**.
4. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 3rd ed. Wiley-Eastern Company, New Delhi, **1990**.
5. L. V. Azaroff, Introduction to Solids, McGraw hill, New York. **1960**.
6. A. R. West, Solid State Chemistry and Its Applications, John Wiley & Sons, **1984**.
7. K. Chakrabarty, Solid State Chemistry, New Age Publishers, **1996**.
8. H. V. Keer, Principles of the Solid State, Wiley Eastern Limited, **1993**.
9. D. M. Adams, Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry, Wiley, **1974**.
10. C. N. R. Rao and K. J. Rao, Phase Transitions in Solids, McGraw Hill, **2010**.
11. A. Earnshaw, Introduction to Magnetochemistry, Academic Press, **1968**

#### Reference Books

1. M. C. Day, and J. Selbin, Theoretical Inorganic Chemistry, Affiliated East West Press Pvt. Ltd. 2nd edition, **1985**.
2. S. F. A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach, Spectrum Academic Publishers, Oxford University Press, **1996**.
3. F. Basolo, and R. G. Pearson, Mechanism of Inorganic Reactions, John Wiley, New York, **1967**.
4. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, 3rd edition, Pearson, **2004**.
5. C. E. Housecraft and A. G. Sharpe, Inorganic Chemistry, 4th edition, Pearson, **2012**.
6. K. F. Purcell and J. C. Kotz, Inorganic Chemistry, Cengage Learning, **2012**.
7. M. C. Day Jr. and J. Selbin, Theoretical Inorganic Chemistry, Literary Licensing, LC, **2012**.
8. G. Wilkinson, R. D. Gillars and J. A. McCleverty, Comprehensive Co-ordination Chemistry, Pergamon Press, **1987**.
9. G. Wulfsberg, Inorganic Chemistry, University Science Books, **2000**.
10. D. M. Adam, Inorganic Solids: An introduction to concepts in solid-state structural chemistry, John Wiley & Sons, **1974**.
11. G. E. Rodger, Inorganic and Solid State Chemistry, Cengage Learning India, Edition, **2002**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	1	2	2	2	3

CO2	2	1	3	3	3
CO3	2	2	3	3	3
CO4	2	1	2	3	3

#### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	15	15	15	15	60
External	10	10	10	10	40
Total	25	25	25	25	100

#### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Punctuality	3	3	3	3	12
Experiment skill	3	3	3	3	12
Performance in Lab	3	3	3	3	12
Maintenance of Observation Records	3	3	3	3	12
Attendance	3	3	3	3	12
Total	15	15	15	15	60

#### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Viva - 01 & 02	5	5	5	5	20
Skill Evaluation	3	3	3	3	12
Record	2	2	2	2	8
Total	10	10	10	10	40

#### Rubric for Internal Assessment

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Punctuality and safety measures	Punctual in coming to the lab and carrying essential safety things	Less punctual and missing any safety things	Ignorant in attending practical and missing 50% safety things	Not attending and no safety things	All
Knowledge about the experiment	Exceptional knowledge about experiment	Considerable knowledge about the experiment	Minimal knowledge about the experiment	Not attended	

<b>Handling of apparatus and recording of observation</b>	<b>Accurate handling of apparatus &amp; Accurate, precise and appropriate reporting and recording the results in SI units</b>	<b>Less proper but careful handling of apparatus &amp; Wrong but appropriate reporting and use of SI units</b>	<b>Proper but careless handling of apparatus &amp; Incorrect way of recording observation</b>	<b>Not attended</b>	
<b>Maintenance of record book</b>	<b>Perfect presentation of record in terms of completeness, neatness, well maintenance and sticking to the dead line of submission</b>	<b>Completing and fine maintenance of record. Adhering to the dead line</b>	<b>Incomplete record</b>	<b>Not submitting</b>	

### MODEL QUESTION PAPER

#### CHE 1071, Solid State and Main Group Chemistry

**Duration: 3 Hours**

**Max. Marks: 60**

**Part – A: Answer ALL questions (4 x 1 mark = 4 marks)**

1. What happens to the electrical resistance of superconductors below critical temperature?
  - a) Increases
  - b) Decreases
  - c) Reaches zero
  - d) Either increases or decreases
2. Identify the incorrect statement from the following:
  - a) In pyrosilicates, one oxygen atom is commonly shared for two tetrahedral units
  - b) In cyclic silicates, one oxygen atom of tetrahedral unit in sharing for cyclic structure
  - c) Sheet silicates share three corners of tetrahedral unit
  - d) Orthoclase is an example three dimensional silicates

**Part – B: Answer ANY FOUR questions (4 x 3 mark = 12 marks)**

1. How Fick's first law of diffusion can be derived?
2. Draw the structure of pentaborane and write its bonding nature. Arrive its STYX number.

**Part – C: Answer ANY TWO questions (2 x 7 mark = 14 marks)**

1.
  - a) Arrive Born-Landé equation. (3 Marks)
  - b) Explain different kinds of diffusion mechanisms. (4 Marks)
2.
  - a) Write a note about the defects in non-stoichiometric compounds. (2 Marks)
  - b) How will you count atoms in three dimensional unit cell? (1 Mark)

**SECTION – B (Coordination Chemistry)**

**(30 marks)**

Note: i) Answers should be brief

ii) Any interchange of sub-questions should be strictly avoided

**Part – A: Answer ALL questions (4 x 1 mark = 4 marks)**

1. The splitting of energy levels due to the interaction of ligands with metal orbitals is known as \_\_\_\_\_.
2. In which one of the following, the transition metal is having a  $d^3$  electronic configuration?
  - a)  $[\text{Fe}(\text{CN})_6]^{3-}$
  - b)  $[\text{Ni}(\text{H}_2\text{O})_6]^{2+}$
  - c)  $[\text{Cr}(\text{NH}_3)_6]^{3+}$
  - e)  $[\text{Co}(\text{H}_2\text{O})_6]^{2+}$

**Part – B: Answer ANY FOUR questions (4 x 3 mark = 12 marks)**

1. Write the important aspects of crystal field theory? What is CFSE?
2. What is spectrochemical series? Explain its application in brief.

**Part – C: Answer ANY TWO questions (2 x 7 mark = 14 marks)**

1.
  - a) Explain the crystal field splitting of d-orbitals in the tetrahedral, octahedral and square planar crystal fields. Draw a correlative diagram exhibiting their relative energies with each other. (3 Marks)
  - a) Calculate the CFSE of the following compounds. (1 Mark)
    - i)  $[\text{Fe}(\text{CN})_6]^{3-}$
    - ii)  $[\text{Ni}(\text{H}_2\text{O})_6]^{2+}$
    - iii)  $[\text{Cr}(\text{NH}_3)_6]^{3+}$
    - iv)  $[\text{Co}(\text{H}_2\text{O})_6]^{2+}$

- c) Explain Jahn-Teller effect? Which configuration(s) ( $d^1$  to  $d^{10}$ ) will have a greater influence due to Jahn-Teller effect? Why? (2 Marks)
- d) What is Irving-William series? (1 Mark)
2. a) What is an Orgel diagram? Explain the Orgel diagram for a  $d^2$  configuration. (3 Marks)
- b) Through the application of Ligand Field Theory, explain the  $\sigma$  and  $\pi$  interactions in octahedral complexes. (3 Marks)
- c) Why  $[V(H_2O)_6]^{4+}$  do not exist as a simple hexaaqua complex? (1 Mark)

### Semester VII

#### CHE1072 - Physical Organic Chemistry & Aromatic Compounds

Credit: 4

Theory

Course Outcomes		Level
CO-1	To describe axial, planar chirality and basics of the asymmetric synthesis	Understand
CO-2	To relate effects of the substituents and sterics in reaction mechanisms	Analyze
CO-3	To state basic principles of aromaticity and the nucleophilic substitutions in such systems	Remember
CO-4	To use nomenclature and synthesis of the fused heterocyclic systems and its properties	Apply

**Advanced Stereochemistry:** Configuration - conformation of cycloalkanes, conformation and reactivity - stereochemistry of allenes, spiranes, biphenyls, molecules with chiral planes, Topicity stereoselective and stereospecific reactions - enantioselective reactions - determination of enantiomeric and diastereomeric excess; double stereo differentiation, asymmetric synthesis, chiral auxiliaries, chiral catalysts and reagents. Resolution – optical and kinetic.

**Physical organic chemistry:** Thermodynamic stability – general relationship between thermodynamic stability and reaction rates – electronic substituent effects on reaction intermediates – kinetic isotope effects – linear free energy relationships – principles of microscopic reversibility – substituent effects – solvent and solvent effects – methods of determination of reaction mechanism.

**Aromaticity:** Criteria of aromaticity - Craig's rule – non-benzenoid aromatic compounds – anti-aromaticity, homoaromaticity – fused-ring systems – hetero aromatic systems. Nucleophilic aromatic substitution reactions – VNS - transition metal- catalyzed aromatic substitution reactions – aromatic substitution reactions involving radical intermediates.

**Advanced Heterocycles:** Nomenclature, heterocyclics with two hetero atoms – fused five and six membered heterocyclics – preparation and reactions of indole, quinoline, isoquinoline and carbazole.

**Prescribed books**

1. F.A. Carey, R.J. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edn, Springer, **2007**.
2. F.A. Carey, R.J. Sundberg, Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th edn, Springer, **2007**
3. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 4th edn, New Academic Science Publisher, **2012**.
4. E. L. Eliel, and S. H. Wilen, Stereochemistry of Organic Compounds, Wiley, **1994**.
5. J.A. Joule, K. Mills, Heterocyclic Chemistry, 5th edn, Wiley-Blackwell, **2010**.
6. R. K. Bansal, Heterocyclic Chemistry, 5th edn, New Age International Private Limited, **2017**.

**Reference books**

1. R.T. Morrison, R.N. Boyd, S. K. Bhattacharjee, Organic Chemistry, 7th edn, Pearson Education, **2010**.
2. S. H. Pine, Organic Chemistry, 5th edn, Tata McGraw Hill, **2008**.
3. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th edn, Cambridge University Press, **2015**.
4. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th edn, Wiley, **2015**.
5. I.L. Finar, Organic Chemistry, Vol I, 6th edn, Pearson Education, **2002**.
6. P. A. Sykes, Guidebook to Mechanism in Organic Chemistry, 6th edn, Pearson Education, **2003**.
7. P. S. Kalsi, Stereochemistry: Conformation and Mechanism, 9th edn, New Age International Private Limited, **2017**.
8. A. R. Katritzky, C. A. Ramsden, J. A. Joule, V. V. Zhdankin, Handbook of Heterocyclic Chemistry, 3rd edn, Elsevier, **2010**.
9. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry, University Science Books, **2005**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	1	1	2	1	1
CO2	1	2	3	2	1
CO3	2	2	1	2	2
CO4	1	3	3	2	1

**Evaluation**

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
<b>Total</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>100</b>

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
<b>Total</b>	<b>12</b>	<b>9</b>	<b>9</b>	<b>10</b>	<b>40</b>

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	
Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Structuring (30 %)	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	
Drafting skill (30 %)	Good language & < 2 % Plagiarism	Good language & < 5 % Plagiarism	< 10 % Plagiarism	> 10 % Plagiarism	

### MODEL QUESTION PAPER

#### CHE1072 - Physical Organic Chemistry & Aromatic Compounds

#### Part A

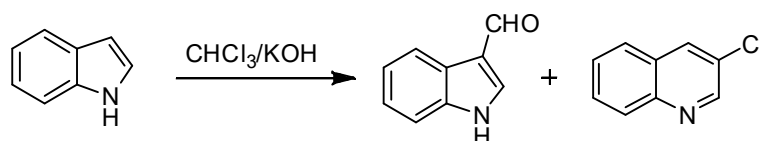
Answer ALL the questions (10 x 1 = 10 marks)

- In gauche butane the dihedral angle ( $\alpha$ ) is -----  
a) 45                      b) 180                      c) 60                      d) 120
- Indoles are -----  
a) acidic                      b) basic                      c) amphoteric                      d) none

#### Part B

Answer any FIVE question (5 x 3 = 15 marks)

- Sketch the mechanism for the following reaction



- What are Meso and Active (dl) compounds? Explain with one example each.

### Part C

Answer ALL the questions (5 x 7 = 35 marks)

1. A) What are **CYCLOPHANE** compounds? Which class of chirality does it belong? Give an example with absolute configuration.

(OR)

- B) i) Define topicity and explain diastereotopicity in detail. (3)

- ii) Predict the conformational analysis of 2-Methylbutane with approximate energy values (4)

(Hint: ethane eclipse conformer = 4.5 k. Cal/mole, Me-Me eclipse energy and gauche energy in butane are 3.6 and 1.2 K. Cal/mole respectively, Me-H eclipse energy is 1.6 k. cal/mole)

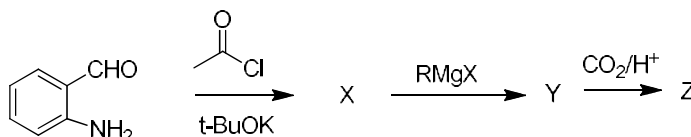
2. A) i) Write about the synthesis of Carbazole.

- ii) How does locking groups affect the stability of conformers in cyclohexane? (4+3)

(OR)

- B) i) Explain the Felkin Anh model of chiral auxiliary.

- ii) Find out X, Y & Z in the following reaction and Sketch the Plausible mechanism.



**Semester VII**  
**CHE1073 - Chemical Kinetics & Group Theory**

**Credit: 4**

**Theory**

Course Outcomes		Level
CO-1	To recall the basic concepts involved in chemical kinetics like reaction rate, order and different types of reactions	Remember
CO-2	To understand the theory and to derive equations involved in heterogeneous catalysis and enzyme catalysis	Understand
CO-3	To evaluate experimental techniques to determine the kinetics of chemical reactions.	Analyze
CO-4	To innovate spectroscopic features of any novel molecules using the concept of GOT	Create

**Chemical Kinetics**

**Introduction:** Reaction rates and order of reactions, determination of order of reactions, complex reactions, reversible, consecutive and concurrent reactions. Reactions of variable order- steady state treatment, free radical reactions.

Fast reactions: relaxation, Flow and Shock methods, Molecular beam methods Flash photolysis, Introduction to femtochemistry.

Theories of reaction rates: Arrhenius equation, Collision cross section and reaction cross section. Steric factor, potential energy surfaces, Thermodynamic formulations of Collision & Transition state theories Comparative study of the theories of reaction rates. Thermodynamic treatment of Reaction rates, Effect of pressure on velocity of gas reactions.

**Molecular Reaction Dynamics:** Heterogeneous catalysis: Unimolecular and bimolecular surface reactions, Langmuir-Hinshelwood and Langmuir-Rideal mechanism-ARRT of surface reactions,

**Enzyme catalysis:** Michelis-Menten equation, effect of pH and temperature on enzyme catalysis. Eley-Rideal and Hinshelwood mechanisms, Lindemann-Hinshelwood mechanism, qualitative idea of RRKM theory, chain reactions, steady state treatment (kinetics of  $H_2-Cl_2$  and  $H_2-Br_2$  reactions), Rice – Herzfeld mechanism.

## Group Theory

**Point Group:** Fundamentals Concept of Symmetry, Matrix representation of symmetry operations. Concepts of groups, molecular point groups, representation of groups, matrix representation of symmetry operations, reducible and irreducible representations, symmetry criterion of optical activity, symmetry restrictions on dipole moment.

**Great Orthogonality Theorem:** Interpretation of character tables, determination of symmetry species for translations and rotations. Transition moment integral, vanishing of integrals, symmetry aspects of molecular vibrations, vibrations of polyatomic molecules

### Applications in Spectroscopy

- I. **IR spectra:** Selection rules for vibrational absorption - Symmetry of normal modes of H<sub>2</sub>O, C<sub>2</sub>H<sub>4</sub>, trans-N<sub>2</sub>F<sub>2</sub>, CHCl<sub>3</sub> and NH<sub>3</sub> using cartesian coordinates and internal coordinates, IR activity.
- II. **Raman Spectra:** Complementary of IR and Raman spectra-determination of the Raman active vibrational modes.
- III. **Electronic spectra:** Selection rules for electronic transition, electronic transitions of simple molecules.

### Applications in chemical bonding

- I. **Transformation of atomic orbitals:** Symmetry adapted linear combinations (SALC), Construction of hybrid orbitals for AB<sub>3</sub>(planar), AB<sub>4</sub>(Td), AB<sub>5</sub>(D<sub>3h</sub>) and AB<sub>6</sub>(Oh) type of molecules
- II. **Ligand field theory:** splitting of d orbitals in different environments using group theoretical considerations
- III. MO diagram for water and ammonia, method of descending symmetry

## Reference Books

1. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, New York, **1988**.
2. F. Daniels and R. A. Alberty, Physical Chemistry, 8th Edition, Wiley, New York, **1994**.
3. P. W. Atkins, Physical Chemistry 8th Edn., Wiley, New York, **2006**.
4. J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, **2000**.
5. K.J. Laidler, Chemical kinetics, 3rd Edn. Harper & Row, **1987**.
6. C. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International, **2005**.
7. D.A. McQuarrie, J. D. Simon, Physical chemistry: A Molecular Approach, University Science Books, **1997**.
8. F. A. Cotton: Chemical Applications of Group Theory, Wiley Eastern, **1985**.
9. P. K Ghosh and P. K Shukla: Atomic Electronic Structure, Prentice Hall of India, **1994**.
10. V. Ramakrishnan and M. S. Gopinathan: Group Theory in chemistry, Vishal Publication, **1986**.
11. D. M. Bishop, Group theory and Chemistry, Dover, **1989**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	1	1	2	1
CO2	2	1	3	2	1
CO3	3	1	3	2	1
CO4	3	1	3	2	1

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
Total	25	25	25	25	100

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
Total	12	9	9	10	40

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
Total	10	14	15	21	60

### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	
Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

#### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Structuring (30 %)	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	
Drafting skill (30 %)	Good language & < 2 % Plagiarism	Good language & < 5 % Plagiarism	< 10 % Plagiarism	> 10 % Plagiarism	

### MODEL QUESTION PAPER CHE1073 - Chemical Kinetics & Group Theory

Duration: 3 Hours

Max. Marks: 60

#### SECTION - A

(Answer all the questions. Each questions carry 1 mark)

1. What is the substrate concentration corresponding to  $V/2$  of enzyme catalysed reactions?
2. Write briefly about the relationships present between symmetry and dipole moment.

### SECTION - B

(Answer any five questions. Each questions carry 3 marks)

1. Derive the collision frequency factor ( $Z_{AB}$ ) and the rate constant ( $K$ ) value using kinetic theory collisions?
2. How to measure the order of the reaction ( $n_c$  and  $n_t$ ) using double logarithmic plots?

### SECTION - C

(Answer the questions. It carries 7 marks)

1. (a) What are the main assumptions made in conventional transition state theory (CTST) ? Derive the rate expression for a biomolecular reaction by considering the motion through the col is determined by loose vibration.  
(or)  
(b) Highlight the importance of flow technique. Explain the plug flow and stirred flow technique.
2. (a) What is Lindemann-Christiansen hypothesis and find out the first order rate co-efficient? Also derive the same by considering the steady state approximation.  
(or)  
(b) Briefly describe the mechanistic steps involved in  $H_2-Br_2$  reaction ? Calculate the  $v_t$  and  $v_p$  of this reaction.

**Semester VII**  
**CHE1074 - Advanced Organic Chemistry Laboratory**

**Credit: 4**

**Practical**

Course Outcomes		Level
CO-1	To organize experiments based on the organic preparations and qualitative analysis	Analyze
CO-2	To use knowledge of the purification techniques	Apply
CO-3	To report separation of two mixture present in the organic compounds	Understand
CO-4	To support on estimation <i>viz</i> volumetric methods	Evaluate

1. Multistep organic synthesis (any four) - conventional synthesis - microwave assisted synthesis - photochemical reactions. Purification of the compounds using column chromatography and characterization of the compounds using spectroscopic techniques.
2. Qualitative Analysis: Separation and analysis of organic mixture containing two components.
3. Estimation of organic compounds:
  - a) Estimation of phenol and aniline - volumetric method.
  - b) Estimation of glucose by Betrand's method.
  - c) Estimation of methyl ketone – iodimetric method
  - d) Determination of iodine and saponification value of an oil sample.

**Prescribed Books**

1. A. I. Vogel, Elementary Practical Organic Chemistry: Small Scale Preparations, Qualitative Organic Analysis, Quantitative Organic Analysis, Pearson Education, **2011**.
2. V.K. Ahluwalia, R. Aggarwal, Comprehensive Practical Organic Chemistry, Universities Press, **2004**.
3. R. K. Bansal, Laboratory Manual in Organic Chemistry, New Age International Pvt. Ltd Publishers, **2009**.
4. F.G. Mann, B.C. Saunders, Practical Organic Chemistry, 4th edn, Pearson Education India, **2009**.
5. A.I. Vogel, A.R. Tatchell, B.S. Furnis, A.J. Hannaford, P.W.G. Smith, Vogel's Practical Organic Chemistry, 5th edn, Pearson Education Ltd, **1996**.

### Reference Books

1. J. Leonard, B. Lygo, G. Procter, Advanced Practical Organic Chemistry, 3rd edn, CRC Press, 2013.
2. P. B. Cranwell, L. M. Harwood, C. J. Moody, Experimental Organic Chemistry, 3rd edn, Wiley-Blackwell, 2017.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	3	2	1	3
CO2	1	3	2	2	3
CO3	1	3	1	2	3
CO4	2	3	1	2	3

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	15	15	15	15	60
External	10	10	10	10	40
Total	25	25	25	25	100

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Punctuality	3	3	3	3	12
Experiment skill	3	3	3	3	12
Performance in Lab	3	3	3	3	12
Maintenance of Observation Records	3	3	3	3	12
Attendance	3	3	3	3	12
Total	15	15	15	15	60

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Viva - 01 & 02	5	5	5	5	20
Skill Evaluation	3	3	3	3	12
Record	2	2	2	2	8
Total	10	10	10	10	40

### Rubric for Internal Assessment

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
<b>Punctuality and safety measures</b>	<b>Punctual in coming to the lab and carrying essential safety things</b>	<b>Less punctual and missing any safety things</b>	<b>Ignorant in attending practical and missing 50% safety things</b>	<b>Not attending and no safety things</b>	<b>All</b>
<b>Knowledge about the experiment</b>	<b>Exceptional knowledge about experiment</b>	<b>Considerable knowledge about the experiment</b>	<b>Minimal knowledge about the experiment</b>	<b>Not attended</b>	
<b>Handling of apparatus and recording of observation</b>	<b>Accurate handling of apparatus &amp; Accurate, precise and appropriate reporting and recording the results in SI units</b>	<b>Less proper but careful handling of apparatus &amp; Wrong but appropriate reporting and use of SI units</b>	<b>Proper but careless handling of apparatus &amp; Incorrect way of recording observation</b>	<b>Not attended</b>	
<b>Maintenance of record book</b>	<b>Perfect presentation of record in terms of completeness, neatness, well maintenance and sticking to the dead line of submission</b>	<b>Completing and fine maintenance of record. Adhering to the dead line</b>	<b>Incomplete record</b>	<b>Not submitting</b>	

**Semester VIII**  
**CHE1081 - Advanced Organometallic & Bioinorganic Chemistry**

**Credit: 4**

**Theory**

Course Outcomes		Level
CO-1	<b>Apply organometallic chemistry principles in catalysis</b>	<b>Apply</b>
CO-2	<b>Gain knowledge in Bioinorganic chemistry and role of metals in biology</b>	<b>Remember</b>
CO-3	<b>Grasp the basics of metalloenzymes and related assessment</b>	<b>Remember</b>
CO-4	<b>Understand magnetic properties of inorganic compounds and material</b>	<b>Understand</b>

**Structure and bonding in organometallics:** 16/18-Electron rule - metal carbonyls – bonding – spectra – metal alkyls, aryls, hydrides and dihydrogen complexes - ligands – metallocenes - electronic structure and bonding in ferrocene - synthesis, physical and spectroscopic properties of metallocenes – fluxional molecules.  $\sigma$ -bonded ligands: metal- phosphines / metal- nitrosyls: structures, reactivity and bonding. Carbenes: N-heterocyclic carbenes, Fischer carbenes, Schrock carbenes, carbynes. Isolobal analogy, metal-metal bond, transition metal clusters. Quintuple bond.

**Reaction mechanism and catalysis:** oxidative addition, reductive elimination, insertion, hydride elimination, abstraction; hydrogenation of olefins, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclooligomerisation, Isomerization reactions, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation, carbonylation, and CH functionalization reactions.

**Bioinorganic Chemistry II: Transport and storage of Metal ions in Biology:** Recapitulation of  $\text{Na}^+$  - $\text{K}^+$  pump) - mechanisms of ion-transport across cell membranes – bleomycin - siderophores (e.g. enterobactin and desferrioxamine) -transport of iron by transferrin - storage of iron by ferritin - biochemistry of calcium as hormonal messenger.

**Metals at the Center of Photosynthesis:** Primary Processes in Photosynthesis – Photosystems I and II - Light Absorption (Energy Acquisition) – Exciton transport (Direct Energy Transfer) – Charge separation and electron transport – Manganese catalyzed oxidation of water to  $\text{O}_2$ .

**Metalloporphyrins/Metalloenzymes:** Dioxygen transport and storage - hemoglobin and

myoglobin: electronic and spatial structures - hemerythrin and hemocyanine – synthetic Oxygen carriers, model systems - blue copper proteins (Cu) - iron-sulfur proteins (Fe) - cytochromes electron transport chain - carbon monoxide poisoning - iron enzymes - peroxidase, catalase and cytochrome P-450, copper enzymes - superoxide dismutase, carboxypeptidase, carbonicanhydrase, vitamin B<sub>12</sub> and B<sub>12</sub> coenzymes, nitrogen fixation. Medicinal bioinorganic chemistry: platinum complexes in cancer therapy – cis-platin and its mode of action – metal toxicity.

**Magnetic properties:**Types of magnetism – Dia –para – ferro and antiferro magnetism. Magnetic properties of free ions – first order Zeeman effect – Second order Zeeman effect – states KT – states<<KT. Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature dependent and temperature independent paramagnetism - Magnetic properties of lanthanides and actinides. Spin crossover in coordination compounds.

### Prescribed Books

1. P.Powell, Principles of Organometallic Chemistry, 2nd ed., Springer, **1998**.
2. K. F. Purcell and J. C.Kotz, Inorganic Chemistry, Saunders Golden Sunburst Series, W.B. Saunders Company, Philadelphia, **1987**.
3. J. E.Huheey, E. A. Keiter,R. L. Keiterand, O. K.Medhi, Inorganic Chemistry - Principles of Structure and Reactivity,4th edition, Pearson Education, **2006**.
4. R. C.Mehrotra, and A.Singh, Organometallic Chemistry, a Unified Approach, New Age International, **2006**.
5. R. H.Crabtree, Organometallic Chemistry of the Transition Metals, 5<sup>th</sup>Ed.Wiley, New York, **2009**.
6. B. D.Gupta, and A. J.Elias, Basic Organometallic Chemistry: Concepts, Syntheses, and Applications of Transition Metals, 1st edition, Universities Press, CRC Press, **2010**.
7. S. J. Lippard and J. M.Berg, Principles of Bioinorganic Chemistry, Panima Publishing Company, New Delhi, **1997**.
8. W.Kaimand, B.Schewederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, New York, USA, **2013**.
9. I.Bertini, H. B.Gray, S. J. Lippardand, J. S.Valentine, Bioinorganic Chemistry, 1st South Asia edition, Viva books Pvt. Ltd., **2007**.
10. S. P. Banerjee, Advanced Inorganic Chemistry, Arunabha Sen, Books and Allied (P) LTD. Volume II, **2015**.
11. C. E.Housecraftand A.G. Sharpe, Inorganic Chemistry, 4<sup>th</sup>edition, Pearson, **2012**.

### Reference Books

1. C.Elschenbroichand A. Salzer, Organometallics: A Concise Introduction, 3<sup>rd</sup>edition, **1999**.
2. N. N.Greenwoodand A. Earnshaw, Chemistry of the Elements, 2nd edition, Elsevier, **2005**.
3. W. L.Jolly, Modern Inorganic Chemistry, McGraw Hill, New York, 2<sup>nd</sup>Edition, **1991**.
4. S. E.Kegley, and A. R.Pinhas, Problems and Solutions in Organometallic Chemistry, University Science Books, Oxford University Press, **1986**.
5. B.Douglas, D. H. McDaniel and J. J.Alexander, Concepts and Models of Inorganic Chemistry, 2nd edition, John Wiley & sons, New York, **2006**.

- M.Bochmann, Organometallics 1: Complexes with transition metal-carbon s-bonds; Oxford Chemistry Primers Series, No. 13, **1994**.
- M.Bochmann, Organometallics 2: Complexes with transition metal carbon  $\pi$  bonds, Oxford Chemistry Primers Series, No.12, **1994**.
- W. Parkins and R. C. Poller, An Introduction to Organometallic Chemistry, Palgrave Macmillan, **1986**.
- Haiduc and J. J. Zuckerman, Basic Organometallic Chemistry, De Gruyter, 1<sup>st</sup> Ed., **1985**.
- R. Hoffmann, Angew. Chem. Int. Ed., Engl. 21, 711-800 **1982**.
- F. A. Cotton, G. Wilkinson, C. A. Murillo and M.Bochmann, Advanced Inorganic Chemistry, 6th ed., A Wiley - Interscience Publication, John -Wiley & Sons, USA, **2007**.
- Chem. Education, 62, No. 11, Bioinorganic Chemistry, State of the Art. **1985**.
- P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5<sup>th</sup> edition, Oxford University Press, **2010**.
- G. L. Miessler, and D. A. Tarr, Inorganic Chemistry, 3rd edition, Pearson, **2004**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	2	2	3	3
CO2	1	1	1	2	3
CO3	3	2	3	3	3
CO4	2	1	2	2	3

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
Total	25	25	25	25	100

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
Total	12	9	9	10	40

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns	3	2	3	2	10

<b>(10 x 1=10 Marks)</b>					
<b>Descriptive (5x 3=15 Marks)</b>		<b>5</b>	<b>5</b>	<b>5</b>	<b>15</b>
<b>Long Answer Qtns (5x 7=35 Marks)</b>	<b>7</b>	<b>7</b>	<b>7</b>	<b>14</b>	<b>35</b>
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

#### Rubric – Seminar

<b>Criteria</b>	<b>Excellent (100 %)</b>	<b>Good (80 %)</b>	<b>Average (60 %)</b>	<b>Poor (50 %)</b>	<b>COs</b>
<b>Quality of content</b>	<b>Complete information with suitable examples</b>	<b>Complete information without suitable examples</b>	<b>Partial information with examples</b>	<b>Partial information without examples</b>	<b>All</b>
<b>Quality of Presentation</b>	<b>Perfect</b>	<b>Good</b>	<b>Average</b>	<b>Poor</b>	
<b>Q &amp; A</b>	<b>Perfect</b>	<b>Good</b>	<b>Average</b>	<b>Poor</b>	
<b>PPT skill</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>	

#### Rubric – Assignment

<b>Weightage Criteria</b>	<b>Excellent (100 %)</b>	<b>Good (80 %)</b>	<b>Average (60 %)</b>	<b>Poor (50 %)</b>	<b>COs</b>
<b>Content (40 %)</b>	<b>Complete information with suitable examples</b>	<b>Complete information without suitable examples</b>	<b>Partial information with examples</b>	<b>Partial information without examples</b>	<b>All</b>
<b>Structuring (30 %)</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>	
<b>Drafting skill</b>	<b>Good</b>	<b>Good</b>	<b>&lt; 10 %</b>	<b>&gt; 10 %</b>	

(30 %)	language &< 2 % Plagiarism	language &< 5 % Plagiarism	Plagiarism	Plagiarism	
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## MODEL QUESTION PAPER

**Course: CHE1081-Advanced Organometallic & Bioinorganic Chemistry**

**Duration: 3 Hours**

**Max. Marks: 60**

**Part - A      Answer ALL the questions      (10 x 1 = 10 marks)**

1. The total number of metal-metal (M-M) bonds in the complex  $[(\eta^4\text{-}(\text{C}_4\text{H}_4)_2\text{Fe}_2(\text{CO})_3)]$  is

- a) 2                                      b) 3                                      c) 0                                      d) 1

2. Based on 18 electron rule, determine the value of "x", for the complex  $[\text{Co}(\text{CO})_3]_x$

- a) +2                                      b) +3                                      c) -2                                      d) -3

**Part- B      Answer any FIVE questions      (5 x 3 = 15 marks)**

1. Identify the number of metal-metal bonds in the following molecules.

- a)  $\text{Fe}_2(\text{CO})_9$                               b)  $[\eta^4\text{-C}_4\text{H}_4)_2\text{Fe}_2(\text{CO})_3]$                               c)  $\text{Fe}_3(\text{CO})_{12}$

2. Write any three different synthetic routes with examples for the preparation of metal carbonyl compound.

**Part-C      Answer ANY FIVE questions      (5 x 7 = 35 marks)**

18 i) What is an 18 electron rule? What are the exceptions to 18 electron rule?

Explain with suitable examples. (3)

ii) Explain the structure and bonding in metal-carbonyl complexes using MO diagram. Also, elucidate how IR spectroscopy will be useful in distinguish the different binding and bridging modes of CO ligand in a metal-carbonyl complexes. (4)

19. i) Write in detail about the structure, synthesis and properties of Fischer carbenes and Schrock carbenes (3)

ii) Explain the following with suitable examples (3)

a) Agostic interaction b)  $\beta$ -hydride elimination c) 1,2-migration

iii) Predict the order of reactivity in metal-alkyls, metal-aryls, metal-alkenes and metalalkynes, justify your answer. (1)

### Semester VIII

#### CHE1082 -Organic Photochemistry & rearrangements

Credit: 4

Theory

Course Outcomes		Level
CO-1	To recognize about the pericyclics in organic chemistry	Understand
CO-2	To state knowledge in the light mediated organic reactions	Remember
CO-3	To examine types of rearrangements in the organic synthesis	Analyze
CO-4	To make a chart on different name reactions and how to apply in the chemical world and research aspects	Apply

**Pericyclic Reactions:** Pericyclic reactions – orbital correlation diagram – FMO. Diels-Alder reactions – 1,3-dipolar cycloaddition reactions – [2+2] cycloadditions and related reactions leading to cyclobutanes – [3,3] and [2,3]-sigmatropic rearrangements – unimolecular thermal elimination reactions. Electrocyclic ring opening and ring closing reactions.

**Organic photochemistry:** Photochemistry of alkenes, dienes and polyenes – photochemistry of carbonyl compounds – photoreductions, photooxidations and - photochemistry of aromatic compounds.

**Molecular Rearrangements:** Benzidine, Sommelet Hauser, Brook, dienone-phenol, Favorskii and Barton rearrangement. Applications of molecular rearrangement reactions in the synthesis of complex organic molecules and natural products

**Selected name reactions in organic synthesis:** Julia olefination; Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction and Ugi reaction, Nazarov cyclization, Robinson annulation; McMurray reaction; Darzens reaction; Mitsunobu reaction; Dotz reaction;

#### Prescribed books

1. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th edn, Springer, **2007**.
2. I. Fleming, Pericyclic Reactions, 2nd edn, Oxford University Press, Oxford, **2015**.
3. S. Sankararaman, Pericyclic Reactions - Applications and Theory, Wiley – VCH, **2005**.

- N. J. Turro, J. C. Scaiano, and V. Ramamurthy, *Modern Molecular Photochemistry of Organic Molecules*, University Science Books, **2010**.
- Sanyal and Sanyal, *Reactions, Rearrangements and Reagents*, 4th edn, BharatiBhawan Publishers and Distributors; **2003**.
- Singh, J., *Photochemistry and Pericyclic Reactions*, 3rd edn, New Age International Publishers, **2012**.

#### Reference books

- R.T. Morrison, R.N. Boyd, S. K. Bhattacharjee, *Organic Chemistry*, 7th edn, Pearson Education, **2010**.
- S. H. Pine, *Organic Chemistry*, 5th edn, Tata McGraw Hill, **2008**.
- M. B. Smith, *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 7th edn, Wiley, **2015**.
- I.L. Finar, *Organic Chemistry, Vol I*, 6th edn, Pearson Education, **2002**.
- I.L. Finar, *Organic Chemistry, Vol II*, 5th edn, Pearson Education India, **2002**.
- P. A. Sykes, *Guidebook to Mechanism in Organic Chemistry*, 6th edn, Pearson Education, **2003**.
- S.M. Mukherjee, S.P. Singh, *Reaction Mechanism in Organic Chemistry*, Trinity Press, **2014**.
- T. H. Lowry, K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd edn, Addison – Wesley Longman Inc., **1998**.
- J. J. Li, E. J. Corey, *Name Reactions for Homologation, Part 1*, Wiley-Blackwell, **2009**.
- B. P. Mundy, M G. Eller, F. G. Favaloro Jr., *Name Reactions and Reagents in Organic Synthesis*, 2nd edn, Wiley-Blackwell, **2005**.
- W. Carruthers, I. Coldham, *Modern Methods of Organic Synthesis*, 4th edn, Cambridge University Press, **2015**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	1	3	2	1
CO2	1	2	3	1	2
CO3	2	3	2	2	1
CO4	1	3	2	3	2

#### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
Total	25	25	25	25	100

#### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5

Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
Total	12	9	9	10	40

#### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
Total	10	14	15	21	60

#### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	All
Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

#### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All

<b>Structuring (30 %)</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>	
<b>Drafting skill (30 %)</b>	<b>Good language &amp;&lt; 2 % Plagiarism</b>	<b>Good language &amp;&lt; 5 % Plagiarism</b>	<b>&lt; 10 % Plagiarism</b>	<b>&gt; 10 % Plagiarism</b>	

### MODEL QUESTION PAPER

#### CHE1082, Organic Photochemistry and Molecular rearrangements

**Duration: 3 Hours**

**Max. Marks: 60**

#### Part – A

Answer ALL the questions

(10 x 1 = 10 Marks)

- Lumiketone rearrangement is given by
  - 4,4-Dialkyl- $\alpha,\beta$  – unsaturated cyclohexenones
  - 4,4-Dialkyl- $\alpha,\beta$  – unsaturated cyclohexanones
  - 4,4-Dialkyl- $\alpha,\alpha'$  – disubstituted cyclohexenones
  - 4,4-Dialkyl cyclohexanones
- Which of the following dienophiles is the most reactive with buta-1,3-diene?

#### Part – B

Answer ANY FIVE questions

(5 x 3 = 15 Marks)

- Predict the stereochemistry of the products formed in the following reactions
- What is Barton reaction? Outline the mechanism.

#### Part – C

Answer ANY FIVE questions

(5 x 7 = 35 Marks)

18. I. Predict the products of the following reactions  
(or)

18. II. Predict the products of the following reactions and comment.

**Semester VIII**  
**CHE1083 - Advanced Quantum Chemistry & Molecular Spectroscopy**

**Credit: 4**

**Theory**

Course Outcomes		Level
CO-1	To apply the advanced quantum chemical methods for solving many body systems.	Apply
CO-2	To solve Schrodinger equation for the simple molecules using perturbation, variation principles and HF methods.	Create
CO-3	To demonstrate the applications of LCAO theory and direct bonding in polyatomic molecules.	Apply
CO-4	To understand pulse sequences in magnetic resonance spectroscopy and apply advanced spectroscopy techniques in the experiments.	Understand

### Quantum Chemistry II

**Potential energy of hydrogen-like systems:** Wave functions and energy of hydrogen like atoms. Orbitals-radial functions - radial distribution functions - angular functions and their plots. The postulate of spin by Uhlenbeck and Goudsmith- Spin orbitals- Construction of spin orbitals from orbitals and spin functions.

Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta ( $L_x$ ,  $L_y$ ,  $L_z$  and  $L^2$ ), commutation relations between these operators. Spherical harmonics as Eigen functions of angular momentum operators  $L_z$  and  $L^2$ . Ladder operator method for angular momentum. Space quantization.

**Schrödinger equation for many electron atoms:** Helium and Lithium atoms.

**Approximation Methods for solving Schrödinger equation:** Born-Oppenheimer approximation, Perturbation theory, Variational methods, Hartree-Fock equations, Self-consistent field methods for solving Hartree-Fock equations, Anti-symmetric wave function, Slater determinant wave function, Molecular Hamiltonian operators.

Valence bond treatment for chemical bonding in molecules - molecular orbitals, Molecular orbital theory for different diatomic molecular systems, photoelectron spectra, SCF-LCAO-MO wave function. Electronic states of diatomic molecules -sp, sp<sup>2</sup> and sp<sup>3</sup> hybrid orbitals. Molecular term symbols, Hückel molecular orbitals, bonding in polyatomic molecules.

**EMR & Origin of spectra:** Nature of EMR, Interaction of EMR with matter, Natural line width and intensity of spectral lines, Classical and quantum chemical approach to absorption of radiation by molecules. Energy levels in molecules. Born Oppenheimer approximation, Population of energy levels.

### Optical Spectroscopy

**Microwave spectroscopy:** Molecular classification and Rotation spectra, Diatomic and polyatomic molecules. Application of Rotation spectra (Bond length, Isotopic mass, dipole moment, isotopic abundance), Non-rigidity of rotor.

**Vibrational spectroscopy:** Vibrational spectra of diatomics& SHO; anharmonicity& Morse potential; Vibration-rotational spectra of diatomics, polyatomic molecules-P,Q,R branches, Dispersive IR & FTIR, Vibration spectra of polyatomic molecules. Normal modes of vibrations of polyatomic molecules, Coupling of rotation and vibration, Parallel and perpendicular bands, Breakdown of Born-Oppenheimer Approximation,

**Raman Spectroscopy:** Polarizability and classical theory of Raman spectrum, Rotational Raman spectra. Vibrational Raman spectra, mutual exclusion principle, Surface enhanced Raman spectra, Resonance Raman,

**Electronic Spectroscopy:** Electronic energy states of molecules. Vibrational structure of electronic bands, Electronic transitions and absorption bands, Selection rules, Electron spectroscopy for chemical analysis (ESCA)-UPS, X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES).

### Reference Books:

1. I. N. Levine: Quantum Chemistry, Prentice Hall India, **1994**.
2. S. N. Datta: Lecture on Chemical bonding and quantum chemistry, **1998**.
3. D. A. McQuairrie: Quantum Chemistry, Oxford University press, Oxford, **1982**.
4. P. W Atkins: Molecular Quantum Mechanics, Clarendon Press, Oxford, **1983**.
5. R. K. Prasad: Quantum Chemistry through Problems and Solutions, New Age International, **1997**.
6. F. L. Pilar: Elementary quantum chemistry, Mc-Graw Hill International, 2nd ed. **1990**.
7. A. K Chandra: Introduction to Quantum Chemistry, Tata McGraw Hill, **1988**.
8. P. W. Atkins, Physical Chemistry, Oxford, London, *6<sup>th</sup> edi*, **1998**.
9. R. Sindhu, Molecular Spectroscopy, Tata McGraw Hill, **1986**.
10. Banwell, Molecular Spectroscopy, Tata McGraw Hill, **1998**.
11. Graebel, Molecular Spectroscopy, Prentice Hall, **1968**.
12. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, **1964**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	2	3	2	2
CO2	3	2	3	2	2
CO3	3	2	3	2	2

CO4	2	2	3	2	2
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### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
<b>Total</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>100</b>

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
<b>Total</b>	<b>12</b>	<b>9</b>	<b>9</b>	<b>10</b>	<b>40</b>

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of	Perfect	Good	Average	Poor	

<b>Presentation</b>					
<b>Q &amp; A</b>	<b>Perfect</b>	<b>Good</b>	<b>Average</b>	<b>Poor</b>	
<b>PPT skill</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>	

### Rubric – Assignment

<b>Weightage Criteria</b>	<b>Excellent (100 %)</b>	<b>Good (80 %)</b>	<b>Average (60 %)</b>	<b>Poor (50 %)</b>	<b>COs</b>
<b>Content (40 %)</b>	<b>Complete information with suitable examples</b>	<b>Complete information without suitable examples</b>	<b>Partial information with examples</b>	<b>Partial information without examples</b>	<b>All</b>
<b>Structuring (30 %)</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>	
<b>Drafting skill (30 %)</b>	<b>Good language &amp; &lt; 2 % Plagiarism</b>	<b>Good language &amp; &lt; 5 % Plagiarism</b>	<b>&lt; 10 % Plagiarism</b>	<b>&gt; 10 % Plagiarism</b>	

## MODEL QUESTION PAPER

### CHE1083: Advanced Quantum Mechanics & Molecular Spectroscopy

**Duration: 3 Hours**

**Max. Marks: 60**

#### SECTION A: (Answer all questions. Each question carries 1 Mark)

1. Calculate the term symbol for ground state Li atom?

2. What is the value of  $100$  of H-atom?

**Section - B (Answer any FIVE questions. Each question carries 3 Marks)**

11. Convert the given Cartesian coordinate  $(1,0,0)$  in the form of polar coordinates?

12. Highlight the importance of volume element to describe the probability density of hydrogen atom?(2)

**Section-C (Answer all questions. Each carries 7 Marks)**

18. (a) Write the electronic Schrodinger equation of H-atom and find out the solution using separation of variable method?

(or)

(b) Describe Perturbation theory for the He atom and find out the lowest order correction to the unperturbed term?

19. (a) (i) Prove that  $E \geq E_0$  for the trial wave function  $\psi = \cos x$ . (ii) Derive the secular determinant of a trial wave function that depends linearly on the variational parameters?

(or)

(b) Explain the Hartree-Fock method for solving the two-electron wave function and list out the limitations of this method?

**Semester VIII**  
**CHE1084 -Physical Methods in Chemistry I**

**Credits 4**

**Theory**

Course Outcomes		Level
CO-1	To explain the electronic transitions and its applications in carbonyl and polyene systems	Understand
CO-2	To learn the principles, instrumentation and functional group identification using IR radiation.	Evaluate
CO-3	To elucidate the structure of organic compounds based on the chemical environment around proton and carbon nuclei.	Analyze
CO-4	To list types of isotopes and material properties.	Remember

**Electronic Spectroscopic:** Basics of UV Spectroscopy, Applications to Organic Molecules, type of transitions, effect of solvent and substituents, Woodward Fieser rule and applications to polyenes, aromatic compounds and carbonyl compounds

**Infra-Red Spectroscopy:** Principle, instrumentation and sampling techniques, types of stretching and bending vibration – Factors influencing the vibrational frequency, vibrational frequencies of alkane, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenol, carbonyl compounds, amines and heterocyclics– related problems.

**NMR Spectroscopy:**  $^1\text{H}$  NMR, Spectral parameters – intensity, chemical shift, multiplicity, coupling constant, factors affecting chemical shift. Analysis of first order and second - order spectra – shift reagents - structure determination of organic compounds by  $^1\text{H}$  NMR spectra. Chemical shifts and coupling constants (spin-spin coupling) involving different nuclei ( $^1\text{H}$ ,  $^{13}\text{C}$ ) interpretation and applications to inorganic compounds. Examples for different spin systems – chemical shifts and coupling constants (spin-spin coupling) involving different nuclei ( $^1\text{H}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$ ,  $^{13}\text{C}$ ) interpretation and applications to inorganic compounds – Effect of quadrupolar nuclei ( $^2\text{H}$ ,  $^{10}\text{B}$ ,  $^{11}\text{B}$ ) on the  $^1\text{H}$  NMR spectra, Satellite spectra.

Systems with chemical exchange - evaluation of thermodynamic parameters in simple systems – study of fluxional behavior of molecules – an elementary treatment of second order spectra – examples – NMR of paramagnetic molecules – isotropic shifts contact and pseudo-contact interactions – Lanthanide shift reagents

**$^{13}\text{C}$  NMR:** Proton coupled; off-resonance decoupled; proton noise decoupled  $^{13}\text{C}$  NMR spectra. Assignment of chemical shifts, additive effect, characteristic chemical shifts of common organic compounds and functional groups, APT, DEPT and INEPT spectra. NMR of common heteroatoms present in organic compounds - 2D NMR techniques  $^1\text{H} - ^1\text{H}$  COSY,  $^1\text{H} - ^{13}\text{C}$  COSY - HMBC, NOESY and INADEQUATE.

**Mass spectrometry:** Elementary idea about mass spectrometry, interpretation of data and solving problems with spectrometric techniques, mass spectra of inorganic and organic molecules

**Microscopic Techniques:** Principles of SEM, AFM, TEM and STM

### Prescribed books

1. R. M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds, John Wiley and Sons. Inc., 6<sup>th</sup> edition, **1997**.
2. W. Kemp, Organic Spectroscopy, 3<sup>rd</sup> edition, MacMillan, **1994**.
3. Jag Mohan, Organic Spectroscopy: Principles & Applications, Narosa Publishers, **2012**.
4. R. S. Drago, Physical Methods for Chemistry, 2<sup>nd</sup> Edition, Saunders College Publishing, **1992**.
5. A. B. P. Lever, Inorganic Electronic Spectroscopy, 2<sup>nd</sup> Sub. Edition, Elsevier Science, **1986**.

### Reference Books

1. Pavia, Lampman and Kriz, Introduction to Spectroscopy, Brooks/Cole Pubs Co, 5<sup>th</sup> edition, **2015**.
2. D. H. Williams and Ian Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill, **1998**.
3. William Kemp, NMR in chemistry: A multinuclear introduction, MacMillan, **1988**.
4. L. D. S. Yadav, Organic Spectroscopy, Kulwer academic publishers, **2004**.
5. F. Gerson and W. Huber, Electron Spin Resonance Spectroscopy for Organic Radicals, Wiley-VCH, 1<sup>st</sup> edition, **2001**.
6. F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, 3<sup>rd</sup> edition, Wiley-Eastern Company, New Delhi, **1990**.
7. J. Wilkins Lewis, R. G., *Modern Coordination Chemistry Principles and Methods*, Interscience Publishers, Inc., **1967**.
8. E. A. V. Ebsworth, Structural Methods in Inorganic Chemistry, 3<sup>rd</sup> edition, ELBS, Great Britain, **1987**.
9. R. A. Scott and C. M. Lukehart, Applications of Physical Methods to Inorganic and Bioinorganic Chemistry, John and Wiley & Sons, LTD, **2007**.
10. E. I. Solomon, A. B. P. Lever, Inorganic Electronic Structure and Spectroscopy, Vol., 2, Applications and Case Studies, Wiley-Interscience, **2006**.
11. D. N. Satyanarayana, Electronic Absorption Spectroscopy, Universities Press, **2000**.
12. R. B. Jordan, Reaction Mechanisms of Inorganic and Organometallic Systems, 3<sup>rd</sup> edition, Oxford University Press, **2007**.

13. C. J. Ballhausen and H. B. Gray, *Molecular Orbital Theory*, Benjamin/Cummings Pub. Co, **1965**.
14. B. N. Figgis and M. A. Hitchman, *Ligand Field Theory and Its Applications*, 1<sup>st</sup> edition, Wiley VCH, **1999**.
15. J. E. Huheey, E. A. Keiter and R. L. Keiter and O. K. Medhi, *Inorganic Chemistry - Principles of Structure and Reactivity*, 4<sup>th</sup> Edition, Pearson Education, **2006**.
16. K. F. Purcell and J. C. Kotz, *Inorganic Chemistry*, Cengage Learning, **2012**.
17. A. Carrington and A. D. McLachlan, *Introduction to Magnetic Resonance*, Harper & Row, New York, **1979**.
18. A. Carrington and MacLachlan, *Magnetic Resonance*, Harper & Row, **1967**.
19. A. Derome, *Modern NMR Technique*, Pergamon, **1983**.
20. Farrar and E. D. Becker, *Pulsed FT NMR Spectroscopy*.
21. Wertz and Bolton, *Electron Spin Resonance*, McGraw Hill.
22. A. E. Derome, *Modern NMR Techniques for Chemistry Research*, Pergamon, **1987**.
23. C. P. Slichter, *Principles of Magnetic Resonance*, Third Edition, Springer-Verlag, **1990**.
24. T. C. Farrar and E. D. Becker, *Pulse and Fourier Transform NMR*, Academic Press, New York, **1971**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	2	2	2	1
CO2	3	2	3	2	2
CO3	3	2	3	2	2
CO4	2	2	2	2	1

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
Total	25	25	25	25	100

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
Total	12	9	9	10	40

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

#### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	
Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

#### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Structuring (30 %)	Perfectly ordered with	Perfectly ordered without	Average structuring with	No order	

	suitable schemes	suitable schemes	suitable examples	
<b>Drafting skill (30 %)</b>	<b>Good language &amp; &lt; 2 % Plagiarism</b>	<b>Good language &amp; &lt; 5 % Plagiarism</b>	<b>&lt; 10 % Plagiarism</b>	<b>&gt; 10 % Plagiarism</b>

## MODEL QUESTION PAPER

### CHE1084 -Physical Methods in Chemistry I

**PART - A**                      **Answer all the questions**                      **(10 x 1 =10 marks)**

1. Choose the correct one of stretching in phenol and alcohol (saturated) from the following,

- (i) C-O stretch ( $\text{cm}^{-1}$ ), Phenol < 3° alcohol < 2° alcohol < 1° alcohol
- (ii) C-O stretch ( $\text{cm}^{-1}$ ), Phenol > 3° alcohol > 2° alcohol > 1° alcohol
- (iii) O-H stretch ( $\text{cm}^{-1}$ ), Phenol > 3° alcohol > 2° alcohol > 1° alcohol
- (iv) O-H stretch ( $\text{cm}^{-1}$ ), Phenol < 3° alcohol < 2° alcohol < 1° alcohol

(a) (i) & (iii), (b) (i) & (iv), (c) (ii) & (iii) (d) (ii) & (iv)

2. As per the fragmentation, pickout the incorrect sentence from the following

- (i) In fragmentation, intense peak due to cleave of the C-C bond ( $\alpha$ ) to the hetero atom
- (ii) In fragmentation, weak peak due to cleave of the C-C bond ( $\alpha$ ) to the hetero atom
- (iii) benzylic cleavage leads to radical site with neutral molecules
- (iv)  $\beta$  cleavage of C-C bond ( $\beta$ ) is helpful to form an aromatic ring

(a) only (i)(b) only(iii)                      (c) both (i & iii)                      (d) (ii, iii & iv)

### PART - B

**Answer any of the five questions**                      **(5 x 3 =15 marks)**

1. Define nitrogen rule and maclafferty rearrangement with example.

2. Write about the  $\alpha$  - cleavage and  $\beta$  - cleavage fragmentation in mass spectroscopy ?

**PART – C**

**(Answer Either OR questions)**

1. (A) Write a notes on (3+2+2)

(a) Nuclear Overhauser effect

(b) Lanthanide shift reagents

(c) Karplus equation

OR

1. (B) (i) Explain in detail about the DEPT spectrum Isopentylacetate.

(ii) Compare and contrast  $^1\text{H}$  and  $^{13}\text{C}$  NMR.

(iii) Although the natural abundance of  $^{12}\text{C}$  is 98.9%, but still it is NMR active.

Why?

(iv) List out the various steps involved in 2D NMR experiments. (3+2+1+1)

2. (A) (i) What is the key difference between SEM and TEM? (2+1+3+1)

(ii) Mention the types of scanning probe microscopy (SPM).

(iii) With neat sketch explain the working principle and applications of AFM.

(iv) Define Quantum tunnelling effect.

OR

2. (B)(i) How to differentiate the meta-diethyl benzene and para-diethyl benzene using IR data. (3+2+2)

(ii) What are the important points to predict amide and amino compounds.

(iii) Compare the electronic spectra of benzene, naphthalene and anthracene.

**Semester VIII**  
**CHE1085 -Advanced Physical Chemistry Laboratory I**

**Credit: 4**  
**Practical**

Course Outcomes		Level
CO-1	To understand the instrumentation methods involved in the experiments	Understand
CO-2	To perform or develop working models	Create
CO-3	To gain the required experimental skills for career development	Create
CO-4	To apply QM methods for modelling simple organic/inorganic compounds for structural optimization and reaction modelling.	Apply

**Part A: List of Wet Lab Chemistry**(Any 10-12 Experiments)

1. *Surface Chemistry*

- a) Verification of adsorption isotherms (Freundlich and Langmuir): charcoal-acetic acid or charcoal-oxalic acid system.
- b) Kinetics & Determination of surface area by adsorption of acetic acid on Charcoal

2. *Phase Diagram*

- a) Determination of the concentration of the electrolyte using CST of phenol-water system
- b) Three Component Liquid Systems: Acetic Acid – Chloroform – Water

3. *Partition Coefficient*

- a) Partition coefficient of benzoic acid between benzene and water.
- b) Molecular formula of copper-ammonia complex by the partition coefficient method

4. *Spectroscopy*

- a) Formation kinetics of Chromium-EDTA complex (Spectrometry)
- b) Simultaneous Estimation of Manganese and Chromium in a Solution of Dichromate and Permanganate Mixture

- c) Photocalorimetric determination of Bimolecular rate constant
5. *Surface Tension*
- a) Determine the surface excess of amyl alcohol.
6. *Potentiometry*
- a) Titration of a strong and weak Acid Mixture with a Strong Base-Potentiometry
- b) Determination of stability constant of silver diammine complex by potentiometric titrations
- c) Dissociation of a weak acid by potentiometric titration
7. *Conductometry*
- a) Verification of Ostwald's dilution law and determination of dissociation constant of weak acid
- b) Conductometric titrations of a mixture of acids Vs strong base
- c) Van't Hoff's factor of benzoic acid between benzene and water
- d) Critical Micelle concentration of surfactant by conductivity measurements
- e) Verification of Onsager's Equation and Determination of Equivalent Conductance at Infinite Dilution of Strong Electrolytes
- f) Conductometric determination of Nickel using DMG
8. *Kinetics*
- a) Second order rate constant for the alkaline hydrolysis of ethyl acetate by conductivity measurements
- b) Arrhenius parameters for the Acid-Catalysed Hydrolysis of Methyl acetate
9. *Viscometry*
- a) Determination of molecular weight of a polymer by viscosity measurements
10. *Additional*
- a) Specific and molar refraction of a liquid by Refractometry
- b) Reversibility of a redox process and determination of concentration of a given solution by cyclic voltammetry
- c) Inversion of Sucrose-Polarimeter

**Part B: List of Computational Chemistry Experiments(Any 3-4 Experiments)**

1. Calculation of electrostatic charges of atoms in organic molecules using population analysis
2. Calculation of Resonance energy of aromatic compounds
3. Calculation of dimerization energy of carboxylic acids
4. Perform the conformational analysis of butane using potential energy scan
5. Find the transition state of simple organic reactions and plot the reaction profile.
6. Determination of heat of hydration of organic molecules.
7. Find the Gibbs free energy of simple gaseous phase reactions and calculate equilibrium constant.
8. Calculation of pKa of simple organic molecules and compare it with experimental values
9. Docking studies involving protein ligand interactions.
10. Calculation of electrophilicity index in hard-soft acids and bases.

**Reference Books**

1. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, **2001**.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn. McGraw Hill, **2009**.

3. B. Viswanathan, Practical Physical chemistry, Viva Pub., **2005**.
4. Saroj Kumar and Naba Kumar, Physical Chemistry Practical, New Central Book Agency, **2012**.
5. A.M. James, F.E. Prichard, Practical Physical Chemistry Paperback, **1974**.
6. J. Foresman & A. Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., **2000**.
7. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems, John Wiley & Sons, **2001**.
8. D. Rogers Computational Chemistry Using the PC, 3rd Edition, John Wiley & Sons, **2003**.
9. Leach, Molecular Modelling: Principles and Applications, 2nd Edn, Longman, **2001**.
10. J. M. Haile, Molecular Dynamics Simulation: Elementary Methods, **2001**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	2	2	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3

#### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	15	15	15	15	60
External	10	10	10	10	40
Total	25	25	25	25	100

#### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Punctuality	3	3	3	3	12
Experiment skill	3	3	3	3	12
Performance in Lab	3	3	3	3	12
Maintenance of Observation Records	3	3	3	3	12
Attendance	3	3	3	3	12
Total	15	15	15	15	60

#### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
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Viva - 01 & 02	5	5	5	5	20
Skill Evaluation	3	3	3	3	12
Record	2	2	2	2	8
<b>Total</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>40</b>

#### Rubric for Internal Assessment

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Punctuality and safety measures	Punctual in coming to the lab and carrying essential safety things	Less punctual and missing any safety things	Ignorant in attending practical and missing 50% safety things	Not attending and no safety things	
Knowledge about the experiment	Exceptional knowledge about experiment	Considerable knowledge about the experiment	Minimal knowledge about the experiment	Not attended	
Handling of apparatus and recording of observation	Accurate handling of apparatus & Accurate, precise and appropriate reporting and recording the results in SI units	Less proper but careful handling of apparatus & Wrong but appropriate reporting and use of SI units	Proper but careless handling of apparatus & Incorrect way of recording observation	Not attended	
Maintenance of record book	Perfect presentation of record in terms of completeness, neatness, well maintenance and sticking to the dead line of submission	Completing and fine maintenance of record. Adhering to the dead line	Incomplete record	Not submitting	

**Semester IX**  
**CHE1091 -Physical Methods in Chemistry II**

**Credit: 4**

**Theory**

Course Outcomes		Level
CO-1	To acquire knowledge on advanced concepts in spectroscopy thereby being able to interpret the spectra and solve the structure of metal complexes.	Remember
CO-2	To discuss the application of electronic spectroscopy to simple coordination compounds and f-block elements	Understand
CO-3	To elucidate the structure of simple organometallic complexes by IR and Raman spectroscopic tools	Apply
CO-4	To depict the advanced spectroscopic tools like EPR, Mossbauer and NQR and its exploitation to express the structure of inorganic complexes	Evaluate

**Electronic Spectroscopy:** Microstates, - terms and energy levels for  $d^1 - d^9$  ions in cubic and square fields – Intensity of bands – group theoretical approach to selection rules - Effect of distortion and spin-orbit coupling on spectra- Orgel and Tanabe-Sugano diagrams – Evaluation of  $10Dq$  and  $\beta$  for octahedral complexes of cobalt and nickel – applications to simple coordination compounds – charge transfer spectra – electronic spectra of  $[\text{Ru}(\text{bipy})_3]^{2+}$ .  
Electronic Spectra of f-block elements.

Optical rotatory dispersion, circular dichroism and Magnetic circular dichroism – applications to metal complexes. Basic principles of inorganic photochemistry.

**Infrared and Raman Spectroscopy:** Group vibrations and the limitations- combined uses of IR and Raman Spectroscopy in the structural elucidation of simple molecules like  $\text{N}_2\text{O}$ ,  $\text{ClF}_3$ ,  $\text{NO}_3^-$ ,  $\text{ClO}_4^-$  effect of coordination on ligand vibrations – uses of groups vibrations in the structural

elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate 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 – Resonance Raman Spectroscopy.

**EPR spectroscopy:**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 VO(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes – Applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions.

**Mössbauer Spectroscopy:**Isomer shifts – Magnetic interactions – Mossbauer emission spectroscopy – applications to iron and tin compounds.

**NQR spectroscopy:**Characteristics of quadrupolar nucleus – effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – applications of NQR spectroscopy.

#### **Prescribed Books:**

1. R. S. Drago, Physical Methods in Inorganic Chemistry, Van Nostrand Reinhold Inc., U. S., **1965**.
2. R. S. Drago, Physical Methods for Chemistry, 2<sup>nd</sup> Edition, Saunders College Publishing, **1992**.
3. A. B. P. Lever, Inorganic Electronic Spectroscopy, 2nd Sub Edition, Elsevier Science, **1986**.
4. J. E. Huheey, E. A. Keiter and R. L. Keiter and O. K. Medhi, Inorganic Chemistry – Principles of Structure and Reactivity, 4th Edition, Pearson Education, **2006**.
5. A. K. Das and M. Das, Fundamental concepts of Inorganic Chemistry, 1<sup>st</sup> Edition, Volume 7, CBS Publishers & Distributors Pvt. Ltd., **2014**.
6. G. Wulferberg, Inorganic Chemistry, University Science Books, **2000**.
7. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part B: Applications in Coordination, Organometallic, and Bioinorganic Chemistry, Wiley-Interscience; 5<sup>th</sup> edition, **1997**.
8. J. Ferraudi, Elements of Inorganic Photochemistry, Wiley, New York, **1988**.

#### **Reference Books**

1. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 3rd ed., Wiley-Eastern Company, New Delhi, **1990**.
2. P. J. Wheatley, The Determination of Molecular Structure, 2nd Edition, Dover Pubns, **1981**.
3. J. and R. G. Wilkins Lewis, Modern Coordination Chemistry Principles and Methods, Interscience Publishers, Inc., **1967**.
4. E. A. V. Ebsworth, Structural Methods in Inorganic Chemistry, 3rd ed., ELBS, Great Britain, **1987**.
5. R. A. Scott and C. M. Lukehart, Applications of Physical Methods to Inorganic and Bioinorganic Chemistry, John and Wiley & Sons, LTD, **2007**.

- E. I. Solomon, A. B. P. Lever, Inorganic Electronic Structure and Spectroscopy, Vol.,2 Applications and Case Studies, Wiley-Interscience, **2006**.
- B. P. Lever, Inorganic Electronic Spectroscopy, 2nd Sub Edition, Elsevier Science, **1986**.
- D.N. Satyanarayana, Electronic Absorption Spectroscopy, Universities Press, **2000**.
- R.B. Jordan, Reaction Mechanisms of Inorganic and Organometallic Systems, 3<sup>rd</sup> Edition, Oxford University Press, **2007**.
- C.J. Ballhausen and H.B. Gray, Molecular Orbital Theory, Benjamin/Cummings Pub. Co, **1965**.
- N. Figgis and M. A. Hitchman, Ligand Field Theory and Its Applications, 1<sup>st</sup> Edition, Wiley VCH, **1999**.
- S.F.A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach, Spectrum Academic Publishers, Oxford University Press, **1996**.
- A. W. Adamson and P. D. Fleischauer, Concepts of Inorganic Photochemistry, Wiley, New York, **1975**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	2	2	2	1
CO2	2	2	2	2	2
CO3	3	2	3	2	2
CO4	3	2	3	2	2

#### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
Total	25	25	25	25	100

#### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
Total	12	9	9	10	40

#### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

#### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	
Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

#### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information with suitable	Complete information without suitable	Partial information with examples	Partial information without examples	All

	<b>examples</b>	<b>examples</b>		
<b>Structuring (30 %)</b>	<b>Perfectly ordered with suitable schemes</b>	<b>Perfectly ordered without suitable schemes</b>	<b>Average structuring with suitable examples</b>	<b>No order</b>
<b>Drafting skill (30 %)</b>	<b>Good language &amp;&lt; 2 % Plagiarism</b>	<b>Good language &amp;&lt; 5 % Plagiarism</b>	<b>&lt; 10 % Plagiarism</b>	<b>&gt; 10 % Plagiarism</b>

### MODEL QUESTION PAPER

#### CHE1091 Physical methods in Chemistry II

##### PART - A

(Answer all the questions)

(10 x 1 = 10marks)

- Find out ground and Russell-Saunders terms for  $V^{3+}$  ion.
  - Compounds like CdS, HgS gives color due to .....
- a) LMCT      b) MLCT      c) d-d transition      d) f-f transition

##### PART – B

Answer any Five Questions

(5x 3 = 15 marks)

- Calculate the number of microstates for the following metal ions.
  - $Cr^{2+}$
  - $V^{2+}$
  - $Ni^{2+}$
- Discuss moderate and strong zero-field splitting EPR transitions of  $V^{3+}$  ion.

##### PART – C

Answer all Questions

(5x 7 = 35 marks)

- 1(A). (i) Define zero field splitting and draw the fine and hyperfine splitting pattern for the high spin octahedral Fe(III) complex in presence of applied magnetic field. (5). (ii) For the nitrogen donor ligands, the nitrogen super hyperfine splitting is commonly noted for the Cu (II) ( $d^9$ ) complexes but it is not usually noted for the analogues oxidovanadium (IV) ( $d^1$ ) complexes. Why? (2)

(OR)

- 1(B). (i) What are the important features that the Mossbauer nuclides should possess?

List at least three nuclei which can exhibit Mossbauer effect. (3)

(ii) What is an “isomer shift”? What are the factors that control isomer shift ?

2(A). (i) Using Mossbauer spectroscopy how the structure or properties of the following molecules can be studied. (4)

a)  $\text{Fe}_3(\text{CO})_{12}$  b)  $[\text{Fe}(\text{II})(\text{phen})_3]\text{X}_2$  and  $[\text{Fe}(\text{II})(\text{phen})_2(\text{NCS})_2]$

(ii) Explain how Mossbauer spectroscopy will be useful to study the nature of chemical bonds and biomolecules such as haemoglobin? (3)

**(OR)**

2(B). (i) Explain the following in detail. (3)

a) Electric field gradient                      b) Nuclear quadrupole coupling constant

(ii) Explain the applications of NQR spectroscopy in elucidating the structures of the following molecules.                      a)  $\text{AlCl}_3$                       b)  $\text{K}_2\text{SeBr}_6$  (3)

(iii) What inferences can be drawn from halogen NQR spectra of the following compounds? a)  $\text{Cs}_2\text{Br}_6$                       b)  $(\text{NH}_4)_2\text{SnBr}_6$  (3)

**Semester IX**  
**CHE1092 -Reagents & Synthetic Strategies in Organic Chemistry**

**Credit: 4**

**Theory**

Course Outcomes		Level
CO-1	To explain importance of asymmetric synthesis in the construction of biologically important molecules	Understand
CO-2	To relate knowledge of organocatalysis and amines in the asymmetric synthesis of natural products.	Analyze
CO-3	To list on various N-heterocyclic carbenes and its applications in the different cascade reactions leading to total synthesis of natural products.	Remember
CO-4	To execute Chiral Bronsted acids to be specific binol derived phosphoric acids and benzoic acids in the asymmetric synthesis and its application in biologically appealing molecules.	Apply

**Protecting and Deprotecting Strategies:** Need for protection and deprotection of functional groups during chemical reactions- protection of hydroxyl, mercapto, amino, carbonyl and carboxylic groups.

**Planning Organic Synthesis:** An introduction to retrosynthesis - Synthons – synthetic equivalent – target molecule, functional group interconversion. Disconnection approach- one

group disconnection- disconnection of alcohols, olefins and ketones. Logical and illogical disconnections. Two group disconnection-1,2, -1,3, 1,4, 1,5 and -1,6 dioxygenated skeletons and dicarbonyls; Umpolung, antithesis, chiron. C-C bond forming reactions, Wieland Mischer ketones (alkylation as well as enamine alkylation). Retro Diels – Alder reactions- Pericyclic reactions- Reterosynthesis of 3, 4, 5, 6 membered heterocycles containing two nitrogens. Designing synthesis: Disconnection approach in Epothilone, Juvabioneandlongifolene,

**Synthetic Reagents:** Use of the following reagents in organic synthesis and functional group transformations: Oxidising reagents: Ozone, CrO<sub>3</sub> DCC, DDQ, lead tetra acetate, phenyl iodoso acetate, dimethyl sulphoxide, SeO<sub>2</sub>, PCC, IBX, Yeast. Phase transfer catalysis – benzyltriethylammonium halides- crown ethers. Reducing reagents: Use of B<sub>2</sub>H<sub>6</sub>, 9-BBN, IPc-BH<sub>2</sub>, NaBH<sub>4</sub>, NaCNBH<sub>3</sub>, LiAlH<sub>4</sub> and Bu<sub>3</sub>SnH; Use of Sn/HCl, Zn/HCl, Hydrazine, Li-NH<sub>3</sub>, Na/alcohol, Pd/H<sub>2</sub> and Raney Ni. Organometallic reagents: Lithiumdialkylcuprate, alkylmagnesiumhalide, alkyl lithium, trimethylsilyliodide, Organoruthenium reagent (Metathesis reactions), Organozinc reagent

#### Prescribed books

1. M. B.Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th edn, Wiley, **2015**
2. F.A. Carey, R.J.Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edn, Springer, **2007**.
3. F.A.Carey, R.J. Sundberg, Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th edn, Springer, **2007**.
4. J.Clayden, N.Greeves, S. Warren, Organic Chemistry, 2<sup>nd</sup> edn., Oxford University Press, **2014**.
5. J. J. Li, E. J. Corey, Name Reactions for Homologation, Part 1, Wiley-Blackwell, **2009**.
6. B. P. Mundy, M .G. Ellerd, F. G.Favaloro Jr., Name Reactions and Reagents in Organic Synthesis, 2nd edn, Wiley-Blackwell, **2005**.
7. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th edn, Cambridge University Press, **2015**.
8. R. O. C. Norman, J. M. Coxon, Principles of Organic Synthesis, 3rd edn, **1993**.
9. P. Wyatt, S. Warren, Organic Synthesis: Strategy and Control, Wiley-Blackwell, **2007**.
10. S. Warren, P. Wyatt, Organic Synthesis: The Disconnection Approach, Wiley, **2008**.
11. E. J.Corey, X. M. Cheng, The Logic of Chemical Synthesis, Wiley-India Private Ltd, **2011**.
12. K. C. Nicolaou, E. J. Sorensen, Classics in Total Synthesis, Wiley-ECH, **1996**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	2	1	3	2	1
CO2	1	3	3	3	2
CO3	2	1	3	2	1
CO4	1	3	3	2	2

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
<b>Internal</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>40</b>
<b>External</b>	<b>15</b>	<b>15</b>	<b>15</b>	<b>15</b>	<b>60</b>
<b>Total</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>100</b>

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Assignment	3	2	2	3	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
<b>Total</b>	<b>12</b>	<b>9</b>	<b>9</b>	<b>10</b>	<b>40</b>

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	
Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered	Perfectly ordered	Average structuring	No order	

	with suitable schemes	without suitable schemes	with suitable examples		
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### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Structuring (30 %)	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	All
Drafting skill (30 %)	Good language & < 2 % Plagiarism	Good language & < 5 % Plagiarism	< 10 % Plagiarism	> 10 % Plagiarism	

## MODEL QUESTION PAPER

### CHE1092 -Reagents & Synthetic Strategies in Organic Chemistry

**PART - A** (Answer all the questions) (10 x 1 = 10marks)

1. Give an example for one carbon synthon.
2. Draw the structure of 9-BBN

**PART – B** Answer any Five Questions (5x 3 = 15 marks)

1. Write a short note on Umpolungreagents.
2. Write any two synthetic uses of LiAlH<sub>4</sub>.

**PART – C** Answer all Questions (5x 7 = 35 marks)

1(A). (i) Write a short note of protection and de-protection strategy used in the synthesis of organic molecule. (5 Marks). (ii) What is DCC? (2 Marks)

(OR)

1(B). (i) What is Wieland Mischer ketones? Give one example. (4 Marks)

(ii) List any three logical retrosynthetic analysis strategy (3 Marks)

### Semester IX

#### CHE1093 -Thermodynamics (Classical & Statistical) & Electrochemistry

Credit: 4

Theory

Course Outcomes		Level
CO-1	To enrich the knowledge about the fundamental concepts of thermodynamics, electrochemistry and statistical thermodynamics.	Remember
CO-2	To recognize the electrochemical ideas at equilibrium and dynamics progress.	Understand
CO-3	To apply the principle of statistical thermodynamics and electrochemical concepts to understand the possibility of existing photovoltaic devices	Apply
CO-4	To develop sensors and energy storage devices based on electrochemical principles	Create

#### Classical Thermodynamics

**Introduction:** Laws of thermodynamics, Entropy- Free Energy-Systems of Variable Compositions - Fugacity and Activity- Fugacity determination (graphical method and Vander Waals equation of state) –Variation of Fugacity with respect to Temperature and Pressure - Maxwell's relations – significance, Partial molar properties – Chemical potential. Concept of absolute entropy and residual entropy

**Thermodynamics of mixing:** Thermodynamic functions of mixing, Clausius Inequality, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law, excess thermodynamic functions

**Chemical Equilibrium:** Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- van't Hoff equations.

**Third law of thermodynamics:** Nernst heat theorem, development of third law of thermodynamics, determination of absolute entropies using third law, entropy changes in chemical reactions.

**Thermodynamics of Irreversible Processes:** Thermodynamics of irreversible processes with simple examples. phenomenological relations. Onsager reciprocal relations - principle of microscopic reversibility. Electrokinetic phenomena. Thermoelectric phenomena.

### **Statistical Thermodynamics**

**Fundamentals of Statistical Thermodynamics:** Thermodynamic probability, stirlings approximation microstate and macrostate, entropy and probability, most probable distribution, Maxwell - Boltzman statistics. Distribution Law-Effect of temperature on distribution, Calculation of most probable velocity, average and mean square velocity, components of velocity, Mean free path, Effusion and diffusion, thermal conductivity and viscosity of gases. Heat capacity of gases - classical and quantum theories, heat capacity of hydrogen

**Partition and Thermodynamic Functions:** Partition function and its relation to thermodynamic properties, translational, rotational and vibrational partition function. Heat capacity of solids: Dulong - Petit law, Einstein's theory and its modification, Debye's theory of heat capacity of solids.

**Quantum statistics:** Bose - Einstein statistics & distribution, example of particles, Bose-Einstein condensation, difference between first order and higher order phase transitions, liquid helium, supercooled liquids. Fermi - Dirac statistics, Fermi-Dirac distribution: examples of particles, application in electron gas, thermionic emission. Comparison of three statistics

### **Electrochemistry**

Activity and Activity coefficient of electrolytes, ionic strength, Debye Huckel theory of strong electrolytes, Debye Huckel limiting law, Mean ionic activity coefficient. Debye Huckeltheory - relaxation and electrophoretic effects, Debye-Huckel-Onsager equation and its derivation. Debye Falkenhagen effect. Wein effect. Ionic activity coefficients of strong electrolytes- Derivation of Debye-Huckel limiting law.

**Equilibrium Electrochemistry:** EMF phenomena, cell potential and its measurement, reference electrodes. Electrochemical cells, concentration cells and activity coefficient determination, liquid junction potential. Determination of solubility. Conductometric, potentiometric and pH metric titrations. Redox indicators and redox titrations.

**Dynamic Electrochemistry:** Electrical double layer, various models of electrical double layer, Electrode polarization. Overpotential, hydrogen and oxygen overvoltage, theories of overvoltage, Butler-Volmer equation for simple electron transfer reactions, Tafel plot and its significance, Corrosion: stability of metals, Pourbaix diagram-Evan diagram-corrosion control and methods for prevention.

**Storage cells:** Lead acid battery, lithium battery, nickel cadmium cell. Fuel Cell. Theory and working of fuel cell. H<sub>2</sub>- O<sub>2</sub> fuel cell, methanol fuel cell, solid oxide fuel cells.

**Electroanalytical Techniques:** Polarography – diffusion current, differential current, supporting electrolyte, polarographic maxima, three electrode system. Amperometry – principles, types and applications. Cyclic voltammetry – principles, applications. Stripping voltammetry.

### **Reference Books:**

1. R.P. Rastogi, R.R. Mishra, An introduction to Chemical Thermodynamics, Vikas publishing house, **2009**.
2. J. Rajaram, J.C. Kuriakose, Thermodynamics, S Chand and Co., **1999**.
3. M.C. Gupta, Statistical Thermodynamics, New age international, **2007**.
4. L.K. Nash, Elements of Classical and Statistical Mechanics, 2<sup>nd</sup>Edn. Addison Wesley, **1972**.
5. F.W. Sears, G.L. Salinger, Thermodynamics, Kinetic Theory and Statistical Thermodynamics, Addison Wesley, **1975**.
6. J. Kestin, J.R. Dorfman, A Course in Statistical Thermodynamics, Academic Press, **1971**.
7. John E. Freund. Modern elementary statistics, **2003**, ISBN-13: 978-0131874398 20.
8. S. P. Gupta, Statistical Methods: S. Chand, **2014**.
9. J. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2B, 2<sup>nd</sup>Edn., Wiley, New York, **1998**.
10. D.R. Crow, Principles and Applications of Electrochemistry, Chapman & Hall, 3<sup>rd</sup>Edn., New York, **1994**.
11. S. Glasstone, Introduction to Electrochemistry, Biblio Bazar, **2011**.
12. B.K. Sharma, Electrochemistry, Krishna Prakashan, **1985**.
13. A.I. Vogel, A Textbook of Quantitative Analysis including Instrumental Analysis, John Wiley & Sons, **1961**.
14. H.H. Willard, J. A. Dean, L.L. Merritt, Instrumental Methods of Analysis, 7<sup>th</sup> Ed., Van Nostrand, **1965**.
15. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8<sup>th</sup> Ed. Saunders College Pub., **2007**.
16. A. J Bard, L.R Faulkner, Electrochemical methods-Fundamentals and applications, 2<sup>nd</sup> Ed., Wiley India Ed.**2004**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	1	1	3	2	2
CO2	3	1	3	2	2
CO3	2	2	3	2	2
CO4	3	2	2	2	2

### MODEL QUESTION PAPER

**Duration: 3 Hours**

**Max. Marks: 60**

#### Part A

**I. Answer ALL the questions**

**(3 X 1 = 3)**

1. Calculate the rotational partition function for CO gas at 27°C, if the moment of inertia is  $14.5 \times 10^{-40}$  g cm<sup>2</sup>. The symmetry number is 1.
2. Write a thermodynamic equation that relates the chemical potential to the composition of a

mixture?

3. Calculate the total number of microstates for 6 identical particles with their occupation numbers 1,2,3 in three states?

**II. Answer any THREE questions**

**(3 X 4 = 12)**

1. What is Fugacity? How to determine the Fugacity of a gas?
2. A solution is prepared by mixing 2 mol of CS<sub>2</sub> and 3 mol of CCl<sub>4</sub> at 298 K and 1 atm. Assuming ideal behaviour calculate DG, DS, DA, DH, DU and DV for the solution process.
3. What is Nernst heat theorem? How does it lead to the enunciation of the Third Law of thermodynamics?
4. Derive the equations which relate the partition function with internal energy and entropy?

**PART B**

**I. Answer ALL the questions**

**(3 X 1 = 3)**

1. Choose the correct and incorrect statement from the following:
  - a) Tafel Plot is the plot of log  $i_0$  and overpotential
  - b) From Tafel plot slope,  $i_0$  can be determined
  - c) From intercept, charge transfer coefficient can be determined
  - d)  $i_c$  is always greater than  $i$  and  $i_a$  is always lesser than  $i$
2. The value of  $\log_{10}K_{sp}$  for Mg(OH)<sub>2</sub> is ----- . Given  $E_0 = -2.36V$
3. a) Arrange the electrode material based on its decreasing oxygen overvoltage:  
Cd, graphite, Au, Pt, Co  
b) Arrange the electrode material based on its increasing hydrogen overvoltage:  
Mo, Bi, Pb, Ni, Hg

**II. Answer any THREE questions**

**(3 X 4 = 12)**

1. a) How will you express the activity of 'm' molal Na<sub>2</sub>SO<sub>4</sub> solution in terms of mean activity coefficient? (Solution necessary) (1 Mark)
2. Derive emf of the cell for the electrolyte concentration cells with transference. (3 Marks)
3. a) Draw the Pourbaix diagram of iron in contact with water and write its significance.

- a. b) Draw Evans diagram and write its significance. (2 Marks)
- (2 Marks)
4. Explain Grahame and BDL double layer models with diagram.
5. Derive charge density based on Debye-Huckel theory.

### Semester IX

#### CHE1094 -Advanced Inorganic Chemistry Laboratory

Credit: 4

Practical

Course Outcomes		Level
CO-1	Ensures the students to acquire knowledge and have hands on experience in multistep inorganic compound synthesis and analysis by using spectroscopic techniques, Separation techniques	Knowledge
CO-2	Apply the knowledge for performing experiment scientifically and safely to enrich the understanding about experiments in lab work	Understand
CO-3	Perform the preparation and purification of simple inorganic complexes by multistep synthesis	Apply
CO-4	Provide hands-on-experience and characterize simple inorganic complexes by cyclic voltammetry and differential pulse voltammetry techniques	Skills

Preparation of the following compounds and their Characterization (Any 10 Experiments)

1. Tetramminecopper (II) sulphate.
2. Potassium trioxalatochromate (III).
3. Potassium trioxalatoaluminate (III).
4. Trithiourecopper (I) chloride.

5. Dibenzyltin dichloride.
6. Nitro and nitrito linkage isomers
7. Mn<sub>3</sub> clusters

1. Synthesis and study of Tris(oxalato)iron(III) potassium salt by Cyclic Voltammetry (CV) and Differential Pulse Voltammetry (DPV), and determination of the following: the formal reduction potential (E<sub>o'</sub>); the number of electrons transferred in the redox process (n); electrochemical reversibility.
2. Synthesis and study of MnIII(Salen)Cl by Cyclic Voltammetry and Differential Pulse Voltammetry (DPV), and determination of the following: the formal reduction potential (E<sub>o'</sub>); the number of electrons transferred in the redox process (n); electrochemical reversibility.
4. Preparation and determination of the effective magnetic moment and number of unpaired electrons in Mn(acac)<sub>3</sub>.
5. Preparation and determination of the aquation rate of [Co(NH<sub>3</sub>)<sub>5</sub>Cl]Cl<sub>2</sub>.
6. Preparation and resolution of the optically active compound [Co(en)<sub>3</sub>]<sup>3+</sup>.
7. Preparation and characterization of (Mesitylene)tricarbonylmolybdenum(0) by solution infrared spectrum.
8. Bioanalytical techniques – Monitoring the cleavage of DNA and protein by metal complexes using Gel electrophoresis techniques – Agarose and PAGE (Demo only).

### Reference Books

1. A. J. Elias, A Collection of Interesting General Chemistry Experiments, Universities Press, Sangam Books Ltd, **2002**.
2. J. D. Woollins, , Inorganic experiments, 3rd edition, Wiley-VCH Verlag GmbH @ Co. KGaA, **2012**.
3. M. Hein, J. N. Peisen and R. L. Miner, Foundations of College Chemistry in the Laboratory, John Wiley and Sons, **2011**.
4. G. S. Girolami, T. B. Rauchfuss and R. J. Angelici, Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, 3rd edition, University Science Books, **1999**.
5. W. L. Jolly, The Synthesis and Characterization of Inorganic Compounds, Prentice-Hall, Inc. **1970**.
6. In-house Laboratory Manual, Department of Chemistry, CUTN.
7. Ghoshal, Mahapatra and Nad, An Advanced Course in Practical Chemistry, New Central Book Agency, **2011**.

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	1	2	2	2	3
CO2	2	3	3	2	3
CO3	3	3	1	2	3
CO4	3	2	3	3	3

### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	15	15	15	15	60
External	10	10	10	10	40
<b>Total</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>100</b>

#### Mapping course outcomes with Internal Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Punctuality	3	3	3	3	12
Experiment skill	3	3	3	3	12
Performance in Lab	3	3	3	3	12
Maintenance of Observation Records	3	3	3	3	12
Attendance	3	3	3	3	12
<b>Total</b>	<b>15</b>	<b>15</b>	<b>15</b>	<b>15</b>	<b>60</b>

#### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Viva - 01 & 02	5	5	5	5	20
Skill Evaluation	3	3	3	3	12
Record	2	2	2	2	8
<b>Total</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>10</b>	<b>40</b>

#### Rubric for Internal Assessment

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Punctuality and safety measures	Punctual in coming to the lab and carrying essential safety things	Less punctual and missing any safety things	Ignorant in attending practical and missing 50% safety things	Not attending and no safety things	All
Knowledge about the experiment	Exceptional knowledge about experiment	Considerable knowledge about the experiment	Minimal knowledge about the experiment	Not attended	
Handling of apparatus	Accurate handling of	Less proper but	Proper but	Not attended	

and recording of observation	apparatus & Accurate, precise and appropriate reporting and recording the results in SI units	careful handling of apparatus & Wrong but appropriate reporting and use of SI units	careless handling of apparatus & Incorrect way of recording observation		
Maintenance of record book	Perfect presentation of record in terms of completeness, neatness, well maintenance and sticking to the dead line of submission	Completing and fine maintenance of record. Adhering to the dead line	Incomplete record	Not submitting	

**Semester X**  
**CHE1101 - Project**

**Credit: 12**

**Practical**

Course Outcomes		Level
CO-1	To design a research-oriented project independently in a particular context.	Create
CO-2	To acquire the skill to write a dissertation, communication skills in a presentation	Evaluate
CO-3	To demonstrate the utility of various software such as ChemDraw, Origin, MS-Office etc.	Apply
CO-4	To prepare a dissertation report with complete follow up of research methodology and to develop the skill of communication in presentation	Create

CO	Program Outcomes				
	PO1	PO2	PO3	PO4	PO5
CO1	3	3	3	3	3
CO2	2	3	3	3	2
CO3	3	3	3	3	3

CO4	3	3	3	3	3
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### Evaluation

	Course Outcomes				Total
	CO-1	CO-2	CO-3	CO-4	
Internal	10	10	10	10	40
External	15	15	15	15	60
<b>Total</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>100</b>

### Mapping course outcomes with Internal Assessment

Component	CO-1	CO 2	CO-3	CO-4	Total
Assignment	2.5	2.5	2.5	2.5	10
Seminar	2	1	1	1	5
Quiz/Test	5	5	5	5	20
Attendance	2	1	1	1	5
<b>Total</b>	<b>11.5</b>	<b>9.5</b>	<b>9.5</b>	<b>9.5</b>	<b>40</b>

### Mapping course outcomes with External Assessment

Component	CO-1	CO-2	CO-3	CO-4	Total
Objective Qtns (10 x 1=10 Marks)	3	2	3	2	10
Descriptive (5x 3=15 Marks)		5	5	5	15
Long Answer Qtns (5x 7=35 Marks)	7	7	7	14	35
<b>Total</b>	<b>10</b>	<b>14</b>	<b>15</b>	<b>21</b>	<b>60</b>

### Rubric – Seminar

Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Quality of content	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	All
Quality of Presentation	Perfect	Good	Average	Poor	

Q & A	Perfect	Good	Average	Poor	
PPT skill	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	

#### Rubric – Assignment

Weightage Criteria	Excellent (100 %)	Good (80 %)	Average (60 %)	Poor (50 %)	COs
Content (40 %)	Complete information with suitable examples	Complete information without suitable examples	Partial information with examples	Partial information without examples	
Structuring (30 %)	Perfectly ordered with suitable schemes	Perfectly ordered without suitable schemes	Average structuring with suitable examples	No order	
Drafting skill (30 %)	Good language & < 2 % Plagiarism	Good language & < 5 % Plagiarism	< 10 % Plagiarism	> 10 % Plagiarism	

### List of Electives

<b>Course Code</b>	<b>Title of the Course</b>	<b>Credits</b>
CHEE01	Principles of Polymer Science	4
CHEE02	Principles of Fluorescence Spectroscopy	4
CHEE03	Asymmetric Catalysis	4
CHEE04	Essentials of Carbohydrate Chemistry	4
CHEE05	Organic Electronics	4
CHEE06	Photochemistry in Molecules and Materials	4
CHEE07	Medicinal Inorganic Chemistry	4
CHEE08	Organic Semiconductors	4
CHEE09	Advances in Polymer Science	4
CHEE10	Advances in Carbohydrate Research	4
CHEE11	Advanced Organic Materials and Catalysis	4
CHEE12	Chemistry of CH Activation	4
CHEE13	Advanced Bio-inorganic Chemistry	4
CHEE14	Principles of Biochemistry	4
CHEE15	Mathematics for Chemists and biologists	4
CHEE16	Electrochemical Energy Systems	4
CHEE17	Fundamentals of Analytical Chemistry	4
CHEE18	Computational Chemistry	4
CHEE19	Supramolecular Chemistry	4
CHEE20	Mathematical methods in Chemistry	4
CHEE21	Organometallics, Catalysis and Inorganic Spectroscopy	4
CHEE22	Physical methods in Chemistry	4
CHEE23	Applications of Computational Methods in Chemistry	4
CHEE24	Chemical Lab Safety and Management	4
CHEE25	Advances in Organic Chemistry	4

CHEE26	Green Chemistry	4
CHEE27	Selected topics in synthetic organic Methods	4
CHEE28	Advanced Topics in Organometallic Chemistry	4
CHEE29	Industrial Chemistry	3
CHEE30	Advanced Organic Nanomaterials	4
CHEE31	Computer software for Chemists	2
CHEE32	Selected Experiments in Applied Chemistry	2
CHEE33	Luminescence Spectroscopy for Advanced Research	4
CHEE34	Research Methodology	4
CHEE35	Chemistry in Nanoscience and Technology	4

\* New electives will be appended based on the availability of course instructor.  
 Electives will be offered based on the individual faculty's availability