Exam Code: 224701 **Paper Code: 1214**

Program: Master of Science (Chemistry) Semester – I

Course Title: Ligand Field Theory

Course Code: MCHL-1081

Time: 3Hours **Max. Marks: 70**

Note: Attempt five questions in all, selecting at least one question from each section. Fifth question may be attempted from any section. Each question carries 14 marks. Students can use non-programmable calculator.

SECTION-A

1. (a) How is group theory helpful in understanding σ and π bonding in square planar transition metal complexes? (7)

   (b) Construct a group multiplication table for C_{3v} point group by taking ammonia as an example. (7)

2. (a) What are the rules relating to the determination of symmetry point group of a molecule? (7)

   (b) Discuss in brief the quantitative splitting of s, p, d and f orbitals in octahedral ligand field. (7)

SECTION-B

3. (a) Illustrate the rules for determining the ground state terms for all configurations using L.S. scheme. (7)

   (b) Discuss the σ and π bonding in square planar complex by constructing molecular orbital diagram. (7)

4. (a) On the basis of molecular orbital theory explain why $[CoF_6]^{3-}$ is paramagnetic whereas $[Co(NH_3)_6]^{3+}$ is diamagnetic in nature. (7)

   (b) What are electron repulsion parameters? Give their types. (7)

SECTION-C

5. (a) Discuss the utility and limitations of orgel diagrams. (7)

   (b) Give an importance of Tanabe-Sugano diagrams. (7)

6. (a) How the selection rules are relaxed in centrosymmetric and non-centrosymmetric molecules. (7)

   (b) How you evaluate strong crystal field term of d^9 configuration in octahedral crystal field using group theory. (7)

SECTION-D

7. (a) Give comments on the spectra of $[Mn(H_2O)_6]^{2+}$ and $CuSO_4.5H_2O$. (7)

   (b) Write a short note on
   (i) Spectrochemical series
   (ii) Nephelauxetic effect (7)

8. (a)Discuss in detail the charge transfer spectra with suitable examples. (7)

   (b) Explain orgel energy level diagram for octahedral and tetrahedral complexes having metal ion with d^2 and d^8 configuration. (7)

Exam Code: 224701 **Paper Code: 1215**

Program: Master of Science (Chemistry) Semester – I

Course Title: Organic Reaction Mechanism-I

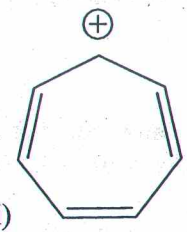
Course Code: MCHL-1082

Time: 3Hours **Max. Marks: 70**

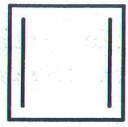
Note: Attempt five questions in all, selecting at least one question from each section. Fifth question may be attempted from any section. Each question carries 14 marks. Students can use non-programmable calculator.

SECTION-A

1. (a) What do you mean by aromaticity. Explain the aromaticity of annulenes and concept of homoaromaticity using appropriate examples? (7)
(b)Explain the conditions for a compound to be an aromatic and antiaromatic. Justify how the following compounds are aromatic/antiaromatic compound?



(i)



(ii) (7)

2. (a) Describe asymmetric synthesis citing its relevance in organic synthesis. Also discuss enantioselective and diastereoselective synthesis of organic compounds with example? (7)
(b) Explain Optical activity in absence of chiral carbon in organic compounds such as Biphenyls, Allenes, and Spiranes citing relevant examples. (7)

SECTION-B

3. (a) Discuss S_N1 and S_N2 mechanism in detail along with their stereochemistry? (7)

(b) Explain with examples neighbouring group participation by sigma and pi-bonds ? (7)

4. (a) Discuss with example kinetic and thermodynamic controlled reaction and difference between two by taking suitable examples? (7)
(b) Discuss in detail the different types of reaction intermediates formed in organic reactions along with their method of isolation? (7)

SECTION-C

5. (a) Discuss S_Ei mechanism and also explain the effect of substrate, leaving group and solvent polarity on the reactivity of electrophilic substitution reactions? (7)
(b) Give detail overview of S_E2 (front and back) and diazo transfer reaction mechanism. (7)

6. (a) Discuss Classical, non-classical and phenonium cations, taking suitable examples? (7)
(b) Explain in detail nucleophilic substitution reactions occurring at allylic and aliphatic trigonal carbon. (7)

SECTION-D

7. (a)Explain reaction, mechanism and synthetic utility of Gattermann Koch reaction and Fries rearrangement reactions? (7)
(b)Discuss concept of ipso attack in aromatic electrophilic substitution reactions. (7)

8. (a)Explain aromatic nucleophilic substitution reaction *via* benzynes mechanism and give evidences in its support? (7)
(b)Explain reaction, mechanism and synthetic utility of Von Richter and Smiles rearrangement? (7)

Exam Code: 224701 **Paper Code: 1216**

Programme: Master of Science (Chemistry) Semester: I

Course Title: Physical Chemistry-Thermodynamics

Course Code: MCHL-1083

Time Allowed: 3 Hours **Max. Marks: 70**

Note: Attempt five questions in all, selecting at least one question from each section. Fifth question may be attempted from any section. Each question carries 14 marks. Students can use non-programmable calculator

Section A

1. Derive Gibbs-Duhem equation. How is it used to obtain relationships of chemical potential with temperature and pressure? Obtain relationships of chemical potential with temperature and pressure? (14)

2. Explain the concept of partial molar properties and describe two methods used to determine them? (14)

Section B

3. (a) Develop an expression based on Debye-Hückel theory for strong electrolytes. (7)

   (b) Using Debye-Hückel theory, demonstrate the relationship between the mean ionic activity coefficient and the ionic strength. (7)

4. What is the concept of activity? How is activity coefficient of electrolytic solutions determined? (14)

Section C

5. (a) Explain the concept of the partition function and derive an expression for internal energy and enthalpy in terms of the partition function. (7)

   (b) Develop an expression for the rotational partition function of an ideal diatomic gas. (7)

6. (a) Explain Fermi-Dirac statistics and discuss its applications in the study of metals. (7)

   (b) Derive an expression for the equilibrium constant of an ideal gaseous mixture using the partition functions of the reactants and products. (7)

Section D

7. Explain the phenomena of microscopic reversibility and Onsager's reciprocal relations. (14)

8. Discuss the following terms:
   i. Non-equilibrium stationary states (7)
   ii. Coupled reactions. (7)

Exam Code: 224701 **Paper Code: 1217**

Programme: Master of Science (Chemistry) Semester I

Course Title: Spectroscopy – A: Techniques for Structure Elucidation of Organic Compounds

Course Code: MCHL-1084

Time Allowed: 3 Hours **Max Marks: 70**

Note: Attempt five questions in all, selecting at least one question from each section. Fifth question may be attempted from any section. Each question carries 14 marks. Students can use non-programmable calculator.

SECTION-A

Q1 a) Discuss with diagrammatic representation Continuous wave measurement techniques in NMR spectroscopy. (7)

b) What do you mean by diamagnetic anisotropy and explain why aromatic protons are more shielded than ethylenic protons. (7)

Q2 a) Write note on nuclear magnetic double resonance and fluxional molecules in NMR spectroscopy. (7)

b) Discuss the role of Lanthanide shift reagent in resolution of NMR spectra. (7)

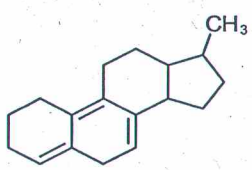
SECTION-B

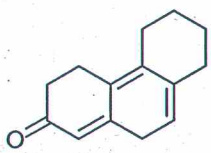
Q3) a) Discuss with diagram the electron impact measurement technique in mass spectroscopy. (7)

b) Explain Frank Condon Principle and its importance in Ultraviolet and Visible Spectroscopy. (7)

Q4) a) Describe the conditions and importance of Retero- Diels – Alder fragmentation in mass spectroscopy with relevant examples. (3)

(b) Calculate wavelength of the following using Woodward- Fieser rules?

(I) 

(II) 

(4)

c) Discuss relative energies of different transitions noticed in UV spectrum of organic compounds and explain the effect of solvent on the U.V. spectrum absorption maxima of organic compounds. (7)

SECTION-C

Q5) a) Describe with example the effect of bond angle and electronic effect on the vibrational frequency of organic compounds. (7)

b) Discuss with examples various types of stretching and bending vibrations that occur in organic compounds in their Infra-red spectrum? (7)

Q6) a) Explain various sampling techniques for handling the different samples in IR spectroscopy. (7)

b) Discuss how you will determine purity of organic compound and study hydrogen bonding by Infra-red spectroscopy. (7)

SECTION-D

Q7) a) An organic compound with molecular weight 54 is transparent to UV spectrum above 200 nm. In the IR spectrum, it shows bands at 3290, 2128 and 620 cm^{-1}• In its 1H NMR spectrum, the following three signals are observed: 81.2 (triple, $J = 7.1$ cps), 1.5 (quartet, $J = 7.1$ cps) and 2.4 (singlet) in the intensity ratio 3 : 2 : 1, respectively. Determine the structural formula of the compound. (7)

b) Molecular formula: $C_9H_{10}0_2$

UV: λrnax 257 nm, Ernax 194.

IR: Significant absorption bands at 3040, 2950, 1740, 1480, 1440 and 1220, 700 and 750 cm-1•

PMR: δ 1.96 (3H, *s),* 5.00 (2H, *s)* and 7.22 (5H, *s).*

MS: Prominent peaks at *mle* 150 (W), 108, 91, 79, 78 and 77. (7)

Q8) a) A compound with molecular weight 130 gave a negative iodoform test.lt absorbs at 292 nm, Emax 16 in the UV spectrum.

It shows significant bands at 3042,2941,2862,2740, 1722, 1605, 1575 and 1462 cm^{-1} in its IR spectrum. In the PMR spectrum, three signals are present at δ 2.73 (multiplet), 7.2 (doublet) and 0.22 (triplet) in the intensity ratio 5 : 2 : 1, respectively. Determine the structural formula of the compound. (7)

b) A compound with the molecular weight 116 gave the following spectral information:

UV: λmax 283, Ernax 22.

IR: A very broad band in the region 2500-3000 cm-1 and a strong band at 1715 cm^{-1}.

PMR: δ 2.12 (3H, *s),* 2.60 (2H, *t),* 2.25(2H, *t)* and 11.1 (lH,s). (7)

Exam Code: 224701 **Paper Code: 1218**

Program: Master of Science (Chemistry) Semester – I

Course Title: Computer for Chemists

Course Code: MCHM-1135

Time: 3Hours **Max. Marks: 20**

Note: Attempt five questions in all, selecting at least one question from each section. Fifth question may be attempted from any section. Each question carries 4 marks.

SECTION-A

1. Write short notes on the following:-
   (a) Character set. (b) Keywords.
   (c) Identifier naming rules. (d) Expressions. **(4)**
2. Define flowchart. What are the various symbols used in flowchart? Write the purpose of each symbol. **(4)**

SECTION-B

3. What are the different types of operators available in C? Explain giving examples. **(4)**
4. Explain if and if-else statement with example. **(4)**

SECTION-C

5. What are the different types of loops in C? Explain giving examples of each type. **(4)**
6. Define functions. What are formal and actual parameters? Explain. **(4)**

SECTION-D

7. Define arrays. How two-dimensional arrays are declared and initialized? Explain giving example. **(4)**
8. Explain terms: break statement, strings, character arrays and array declaration. **(4)**