

- c) Find the value of K after the following program segment is executed. [2]
- ```

 K=0
 DO 30 I=5, 25, 3
 K=K+1
 IF(K.GT.12)GO TO 36
30 CONTINUE
36 K=2*K

```

- Q.2 Write a FORTRAN program to evaluate the value of  $\int_a^b \frac{1}{1+x^2} dx$  by using Simpson's 1/3 rule. [10]

OR

Write a FORTRAN program to evaluate the mean and standard deviation of N numbers  $a_1, a_2, a_3 \dots \dots a_N$ . [10]

- Q3. What do you mean by a basis set? Which properties must be possessed by a function for being a basis set? Define the equations of the Slater Orbital and Gaussian Orbital for 1s orbital and show that  $\phi_{1s} = S_{1s}^{STO}(0,1.24) = 0.779$ . Discuss how STO (Slater type Orbital) is different from GTO (Gaussian type Orbital).

[1+1+4+4=10]

OR

What is computational Chemistry? Discuss in brief the Gaussian and GaussView Software and write the detail of Gaussian input and output file with H<sub>2</sub>O as an example. [1+2+7=10]

- Q4. Write a brief account on Hartree-Fock Model and discuss how Hartree-Fock Self Consistent Field Method estimates a wavefunction.

[5+5=10]

OR

Discuss on Single Point Energy (SPE) Calculation and Configuration Interaction (CI).

[5+5=10]

M.Sc. Chemistry 2<sup>nd</sup> Semester Examination, 2021(June)  
Dhanamanjuri University  
G.P.Women's College

**CHE-508**  
(Inorganic Chemistry)

**Full Marks: 40**

The figures in the right-hand corner indicate full marks for the questions.

Symbols used in the questions have their usual meanings.

**Answer any four questions.**

1. Discuss the Spectrophotometric method for the determination of stability constants of complexes. [10]
2. How does the nature of the central metal ion affect the stability of the complexes? [10]
3. Give detailed information about Spin crossover with suitable examples. [10]
4. (a) What are the basic principles of Gouy's balance method of measuring magnetic susceptibility of a sample? Why does the meniscus level rise up and fall down in presence or absence of an external uniform magnetic field?  
(b) Find out general Valence Shell E.C. of the following terms  
(I) 1D (II) 3P (III) 1S (IV) 3D [6+4=10]
5. Discuss the complementary and non-complementary two electron transfer reactions giving suitable examples. [10]
6. Describe the various reactions of Ferrocene which establishes its aromatic character. How can you say that the aromaticity of Ferrocene is more than that of Benzene? [10]
7. (a) Give two methods of preparation of transition metal carbonyls.  
(b) Discuss the bonding in metal carbonyls. How does IR spectroscopy help in explaining bonding in metal carbonyls? [4+6=10]

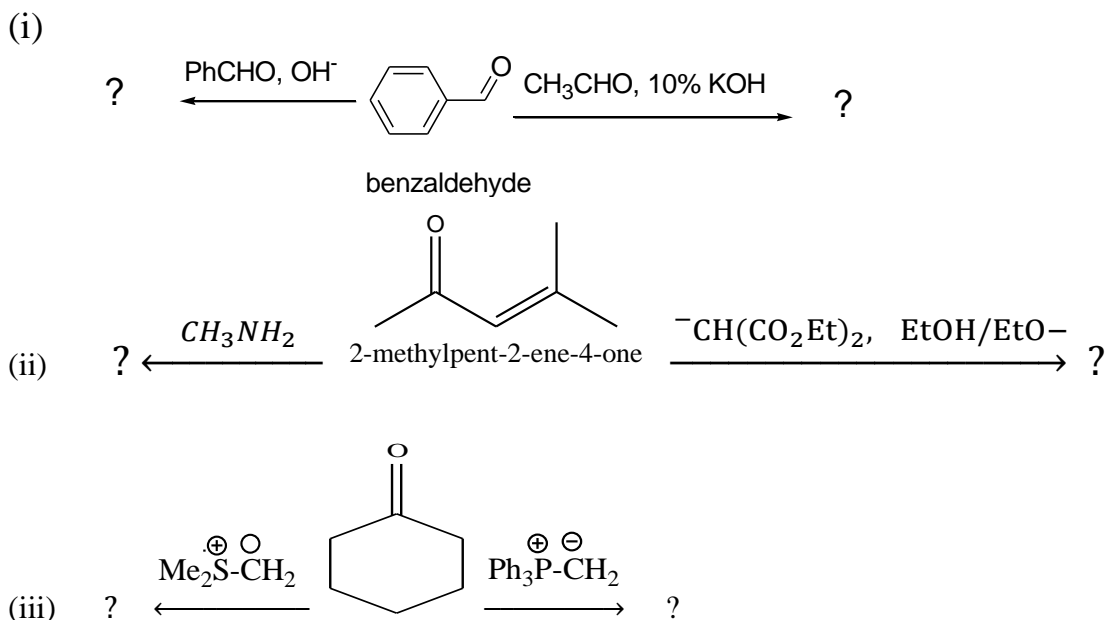
**CHE-509**  
 (Organic Chemistry)

**Full Marks: 40**

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**Answer all questions.**

1. Predict the products formed in the following reactions detailing the reaction mechanism also: [3+4+3=10]



**OR**

(a) What is umpolung effect? Describe a reaction which demonstrates the umpolung effect using 1,3-dithiane as a reagent. Explain its synthetic application by giving an appropriate example. [1+2+1=4]

(b) Using examples, give the reaction mechanism of the following name reactions:  
 (i) Michael Addition  
 (ii) Dieckmann Condensation  
 (iii) Crossed-Aldol Condensation

[2+2+2=6]

2. (a) Give one method of preparation of the following compounds: [2+2+2=6]
- Pyrazole
  - 2-amino-4-methyl thiazole
  - oxetane

(b) Discuss the electrophilic substitution reaction of imidazole with chloromethane giving reaction mechanism. [4]

**OR**

(a) Discuss the ring strain developed in 3- and 4- membered heterocyclic compounds. How does the ring strain influence the reactivity and ring openings of these heterocycles? Discuss the biological importance of  $\beta$ -lactam antibiotics and lactones.

[2+2+2=6]

(b) What happens when (give reactions):

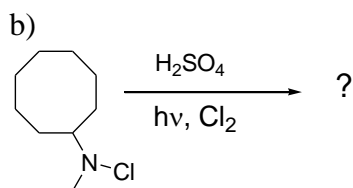
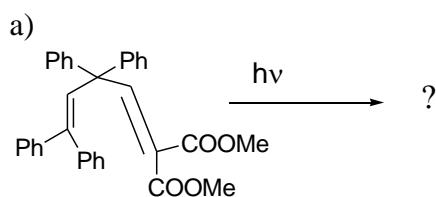
- Aziridine reacts with ammonia?
- Imidazole reacts with hydrogen peroxide?

[2+2=4]

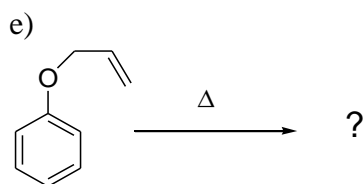
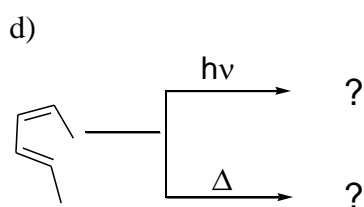
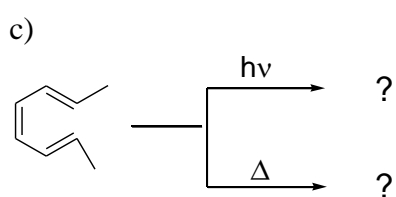
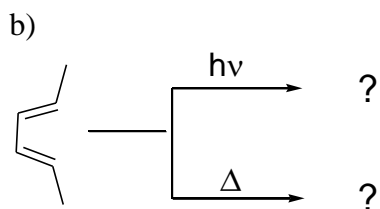
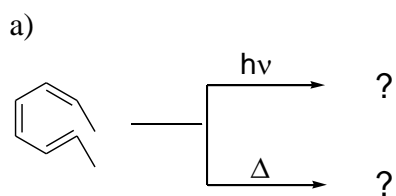
3. Write the short note on the following reactions. [5 + 5 = 10]
- Paterno Buchi reaction
  - Norish type II reaction

**OR**

Write the product of the following reactions with plausible mechanism. [5 + 5 = 10]

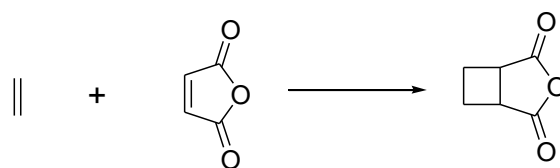


4. Write the major product of the following reaction with proper stereochemistry whenever it required. [2x5=10]



**OR**

(a) Illustrate the following cycloaddition reaction is photochemically allowed and thermally forbidden by using frontier molecular orbitals.



(b) According to Woodward-Hoffmann correlation diagram, 1,3 butadiene electrocyclic interconversion through disrotatory motion in photochemical condition is feasible. Justify it.

(c) Write a short note on Cope reaction.

[4 + 4 + 2 = 10]

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**CHE-510**  
(Physical Chemistry)

**Full Marks: 40**

The figures in the right-hand corner indicate full marks for the questions.

Symbols used in the questions have their usual meanings.

**Answer any four questions.**

1. (a) Write the Schrodinger wave equation in Cartesian co-ordinates and solve the equation for  $\theta$  and  $\phi$  by converting it into polar co-ordinates.  
(b) Write the expression for spherical harmonics  $Y_{l,m}(\theta, \phi)$ .

[8+2=10]
2. Taking the ground state Helium atom, explain Pauli's antisymmetric wave function. Express the wave function in the Slater determinant form.

[7+3=10]
3. (a) Show that for a many electron system only the wave function taken as product and not as sum of H-like orbital is acceptable.  
(b) Write a brief note on Slater type orbitals.

[7+3=10]
4. (a) Define weight average and number average molecular mass of a polymer.  
(b) Describe in brief the determination of molar mass of a sample of polymer by light scattering or viscosity measurement method.

[1+1+8=10]
5. (a) What is kinetic chain length? Show that the kinetic chain length of a cationic polymerization is first order with respect to monomer.  
(b) Calculate the most probable end-to-end distance of a polymer chain  $C_{20}H_{42}$ , given that the C-C bond length is 154 pm and the bond angle is  $109^{\circ}28'$ . (Also given that  $\cos 70^{\circ}32' = 0.333$ ).

[1+6+3=10]

6. (a) Which of the following molecules show rotational spectra and why?

HCl, CS<sub>2</sub>, CCl<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>

(b) Show that lines in the rotational spectrum of a diatomic molecule are equispaced under rigid rotator approximation.

(c) What is the frequency of the rotational line shown by a diatomic molecule having the moment of inertia value of  $16.5 \times 10^{-40} \text{ g cm}^2$ , the excited molecule being in quantum state  $J=2$ .

[2+4+4=10]

7. (a) What are the selection rules for the rotational transition of a diatomic molecule.

(b) Explain why only those molecules having permanent dipole moment exhibit rotational spectra.

(c) What are the degeneracies of the following diatomic rotational energy level?

(i)  $\frac{h^2}{4\pi^2 I}$

(ii)  $6 \frac{h^2}{4\pi^2 I}$

[2+4+4=10]



M.Sc. Chemistry 2<sup>nd</sup> Semester Examination, 2021(June)  
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**OPE-011**  
(Nanomaterials and Nanotechnology)

**Full Marks: 40**

The figures in the right-hand corner indicate full marks for the questions.  
Symbols used in the questions have their usual meanings.

**Answer all questions.**

- Q.1 What are nanomaterials? How they are classified? Give examples. (2+6+2=10)  
Or  
Write a brief history and development of nanomaterials and nanotechnology. (10)
- Q.2 Explain the phenomena of conductivity and magnetism in nanomaterials. (10)  
Or  
Explain the following terms related with nanomaterials  
i) Surface Plasmon  
ii) Self-assembly (5x2 =10)
- Q.3 Explain the characterization of nanoparticles using XRD and TEM (10)  
Or  
How would you characterize nanoparticles using UV-visible and DLS? (10)
- Q.4 Briefly describe the advantages of nanocatalysis? Explain the role of photocatalytic nanomaterials on water splitting and band gap tuning. (3+7=10)  
Or  
What is the potential impact of nanotechnology? Explain the role of it in targeted drug delivery and hyperthermia? (4+6=10)