Mahindra University Hyderabad
École Centrale School of Engineering
End-semester Regular Examination
(Batch 2022)

UM

Program: B. Tech Branch: CAM Year: I Semester: II

Subject: Chemistry II (Fractal) (CH 1204)

Date: 12/06/2023 Start Time: 10.00 AM

Time Duration: 3.0 Hours Max. Marks: 100

Instructions

1. Answer all questions.
2. No clarifications will be entertained during the examination.
3. If any information is missing, make appropriate assumptions and proceed.

PART-A

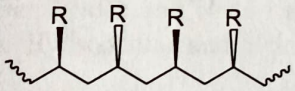
Q1. (Marks: [4+4+2=10])

(A) What do you understand by following types of polymers?
(i) homopolymers (ii) copolymers

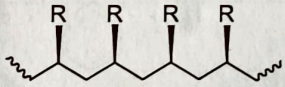
(B) Describe addition (or chain growth) polymerization method?

(C) Identify isotactic polymer and syndiotactic polymer from the following structures.

(i)



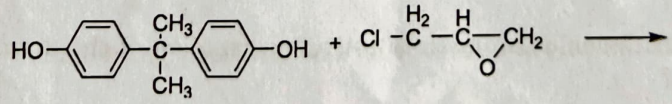
(ii)



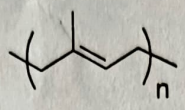
Q2. (Marks: [4+3+3=10])

(A) Show the mechanism for (i) initiation (ii) propagation, and (iii) termination steps of free radical polymerization.

(B) What kind of epoxy resin product is obtained by following polymerization reaction?

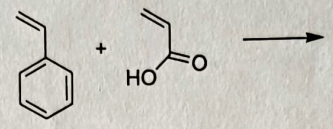


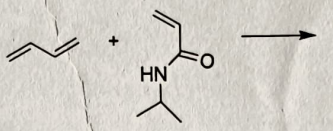
(C) Show the vulcanization process in rubber by taking an example of following natural polymer ? poly(isoprene).



Q3. (Marks: [4+3+3=10])

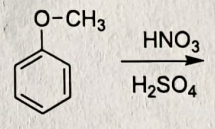
(A) Draw the structure of the polymer products in the following reaction.

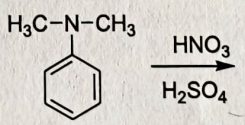
(i) 

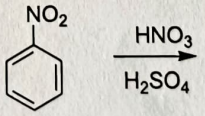
(ii) 

(B) What is called (i) electrophiles, and (ii) nucleophiles?

(C) Draw the structures of products for the following nitration reactions.

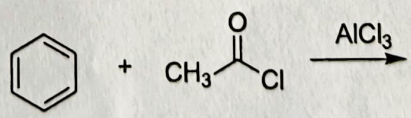
(i) 

(ii) 

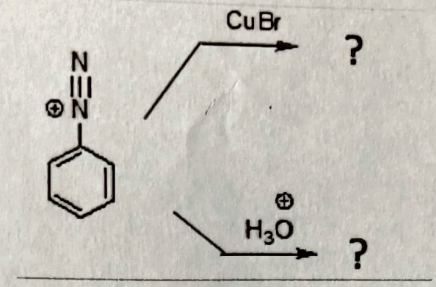
(iii) 

Q4. (Marks: [3+2+5=10])

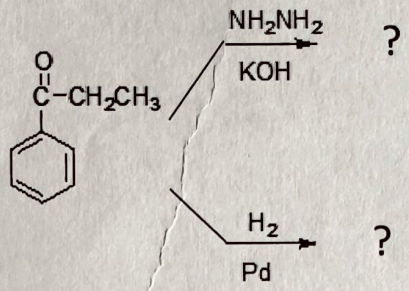
(A) Identify the name of following acylation reaction, and find out its product.



(B) The following nucleophilic aromatic substitution reaction of the diazonium ions will lead to which product?



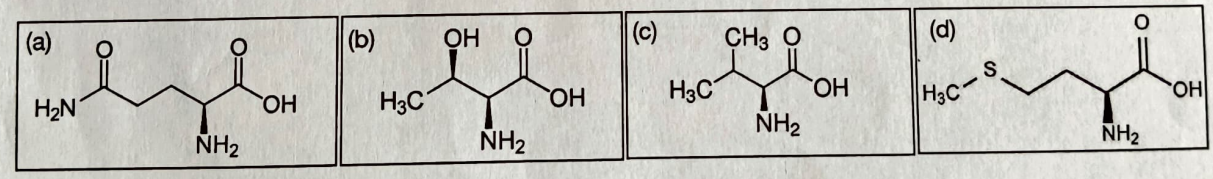
(C) Identify the name of the reaction and the product structure for the following.



PART-B

Q5. (Marks: [8+2=10])

(i) Identify the amino acid residues given below, and write their names using the three-letter code. Classify them into two groups: Hydrophobic and hydrophilic.



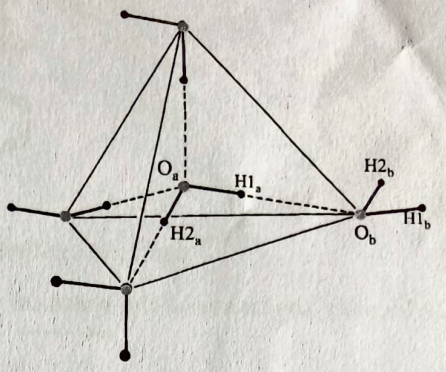
(ii) Give examples of each chemical interactions that stabilize protein structures: (a) Covalent, and (b) Non-covalent

Q6. (Marks: [5+5=10])

Draw the structures of the following peptides, and label torsion angles Phi (Φ) and Psi (Ψ): (a) Gly-Ala, and (b) Ala-Gly

Q7. (Marks: [3+2+10+5=20])

Here a three-dimensional tetrahedral network of water molecules is shown. Oxygen atoms (shown in grey) are situated at the centre and at the vertices of a regular tetrahedron. Answer the following questions:



(i) Write down the expressions for the two types of nonbonded interaction potentials between two oxygen atoms $H1_a$ and O_b.

(ii) Can you imagine how many such van der Waals, V_{ab}^{vdW} and electrostatic, V_{ab}^{ele} interaction terms will arise for two interacting water molecules?

(iii) Derive the force (z-direction) acting on atoms interacting via Lennard-Jones potential.

(iv) Now, calculate the Lennard-Jones force (z-direction) acting on $H1_a$ and O_b atoms separated by 2.7 Å. [Given: $\epsilon_{OH} = -0.1$ kcal/mol, $\sigma_{OH} = 2.7$ Å]

Q8. (Marks: 10)

Consider a system of distinguishable particles with five microstates with energies $0, \epsilon, 2\epsilon, 2\epsilon$ and 3ϵ in equilibrium with a reservoir at temperature T = 3000 K. Find the partition function of the system. [Given: $\epsilon = 1.0$ eV, Boltzmann constant (k_B) = 1.381×10^{-23} J K^{-1}, 1 eV = 1.602×10^{-19} J]

Q9. (Marks: [5+5=10])

(i) Match the following:

Protein structures	Structural elements
Primary	Loops, turns
Secondary	Backbone
Tertiary	Monomer, dimer
Quaternary	α-helices, β-sheets

(ii) Fill in the blanks with appropriate answer.

(a) There are _____ different naturally occurring amino acids.

(b) Properties of amino acids are determined by their specific _____.

(c) Time-step in a typical MD simulation is _____.

(d) Velocity Verlet integration algorithm is _____.

(e) In microcanonical ensemble each microstate exists with _____ _____.