

## Indian Association for the Cultivation of Science (Deemed to be University under de novo Category)

Master's/Integrated Master's-PhD Program/Integrated Bachelor's-Master's Program/PhD Course

Mid-Semester Examination-Spring 2025

Subject: Structure, Spectroscopy and Kinetics Full Marks: 25

Subject Code(s): CHS1201

Time Allotted: 2 h

## Part I: Physical Chemistry [12.5 marks]

1. In vibrational spectroscopy, what is a) fundamental transition and b) hot band transition? How can you differentiate between the two in a spectrum. [2.5]

2. Calculate the ratio,  $N_1/N_0$ , of molecules in the v = 1 and v = 0 vibrational states for CO, at 25.0 °C. Assume a harmonic oscillator with  $\omega_e$  = 2169.8 cm<sup>-1</sup> [Hint: at 25.0 °C, kT = 207.2 cm-1] [1.5]

J3. Explain predissociation with diagram.

[2.5]

J4. Discuss the basic principles of LASER operation.

[3.5]

5. The microwave spectrum of a molecule yields 3 rotational constants, such that:  $A \neq B \neq C \neq 0$ . The molecule(s) is/are:

a) CO<sub>2</sub> b) CO c) CH<sub>4</sub> Justify your choice with proper explanation.

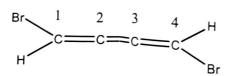
d) BCl<sub>3</sub> e) CH<sub>2</sub>==CHCl

[2.5]

## Part II: Organic Chemistry [12.5 marks]

1. Consider the following molecule and answer the subsequent questions

[5x0.5]



Ji) Identify the state of hybridization of the carbon atoms (C1 to C4)

Ji) Find the maximum number of atoms lying in one plane

A. /iii) Can this molecule show stereoisomerism? If yes, indicate the type of stereosomerism (enantiomerism or diastereomerism)? A. /iv) Is this molecule resolvable? whether resolution is possible.

Provide reasons for your answers to iii) and iv)

2. The structure of amino acid lysine when kept at pH 2 is shown below. Indicate the order of removal of the acidic hydrogens when the pH is gradually raised. [2]

- 3. Draw the possible canonical forms for E-2-methoxy-1-nitroethylene and identify the most stable structure(s) citing reasons. [2]
- Mhich one amongst the following carbocations will have the highest hyperconjugative stabilization? Justify. [2]

$$H_3C$$
 $H_3C$ 
 $H_3C$ 
 $H_3C$ 
 $H_2C$ 
 $CH_3$ 
 $H_2C$ 
 $CH_3$ 
 $CH_3$ 
 $CH_3$ 

5. Answer the following questions:

[4]

- A) Explain the difference between asymmetric and dissymmetric molecules
- B) in terms of symmetry elements, what is the minimum condition for chirality for a molecule?
- C) Find the number of sigma planes in the following structures



D) Define a stereogenic center. Identify the stereogenic centres in the following molecules:

HO 
$$\frac{1}{2}$$
 H
HO  $\frac{3}{4}$  H
HO  $\frac{4}{6}$  H
H  $\frac{5}{7}$  H
H  $\frac{6}{6}$  OH