



ELIZADE UNIVERSITY,
ILARA-MOKIN, NIGERIA

FACULTY: BASIC & APPLIED SCIENCES

DEPARTMENT: BIOLOGICAL SCIENCES

FIRST SEMESTER EXAMINATION

2020/2021 ACADEMIC SESSION

COURSE CODE: EMT 509

COURSE TITLE: STRUCTURAL ELUCIDATION OF ORGANIC POLLUTANTS

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21/10/2021

COURSE UNIT(S): 3 UNITS

DURATION: 3 HOURS

HOD's SIGNATURE

NAME:

MAT. No:

INSTRUCTIONS:

ANSWER ANY FOUR QUESTIONS

USE THE TABLE OF VALUES GIVEN WHERE NECESSARY.

1. Given that (A) is an organic compound with molecular formula $C_4H_8O_2$. Use the information provided to elucidate its structure.

(a) Determine its Double Bond Equivalent (DBE) and hence, comment on its structure if it has no significant absorption of Ultraviolet-Visible (UV) radiation.

(b) Infra-red (IR) absorption at: 3500 cm^{-1} , 2980 cm^{-1} and 1725 cm^{-1} .

(c) Nuclear Magnetic Resonance (NMR) data:

δ values 2.20, 3H, s; 2.40, 1H, t; 4.60 removed by D_2O shake, 1H, s

(d) (A) reacts to form a compound (M) with the following information:

IR: Band at 3500 cm^{-1} disappears and band at 1725 cm^{-1} moves to 1690 cm^{-1} .

UV: Compound now has a strong absorption at 215 nm.

NMR: Signals at 2.40, 3.60 and 4.60 disappear and δ 5.0, 3 H appears.

IR: Band at 1640 cm^{-1} appears.

Mass Spectroscopy (MS) data: $m/z = 43$; $m/z = 63$ and $m/z = 31$.

(20 Marks)

2. a. An Ultra-violet light has a wavelength of 200 nm. Calculate the:

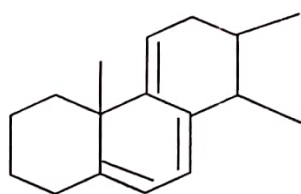
(i) amount of energy absorbed by one molecule that interacts with this light

(ii) frequency of the light ($c = 3 \times 10^8\text{ m.s}^{-1}$; $h = 6.6 \times 10^{-34}\text{ J s}$)

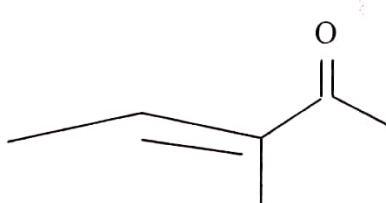
b. Explain the following terms: (i) Chromophore (ii) Blue shift

c. List two factors that influence the relative energy of absorption of UV radiation by a molecule.

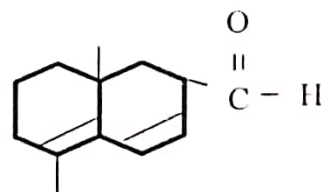
d. Given molecules (B), (C) and (D), predict λ_{max} for $\pi \rightarrow \pi^*$ absorption band in the UV spectrum.



(B)



(C)



(D)

(15 Marks)

3. a. Write on chemical warfare and coevolutionary arms race.

b. State the number of signals that will be observed in the ^1H NMR of the following:

(i) $\text{CH}_3\text{CH}_2\text{CCH}_2\text{CH}_3$ (ii) $\text{C}(\text{CH}_3)_4$ (iii) $\text{CH}_3\text{CHCH}_2\text{Br}$ (iv) $(\text{CH}_3)_2\text{C}=\text{CH}_2$

c. An NMR signal is observed at 100 Hz down field from TMS using a 60 MHz instrument. What is the position of the signal in δ value?

d. Compound (E) has molecular formula $\text{C}_3\text{H}_6\text{O}_2$. NMR spectrum of (E) has the following:

NMR δ 2.00, singlet; δ 3.75, singlet. Area ratio 14.2:13.9. Deduce its structure.

(15 Marks)

4. a. Highlight in details, the steps involved in classical method of elucidating the structure of organic compound.

b. State four factors that affect absorption frequency in Infra-red (IR) spectroscopy.

c. How can you differentiate between the following pair of compounds by means of IR spectroscopy?

(i) PhCOCH_3 and PhCOOCH_3

(ii) $\text{CH}_3\text{CH}_2\text{CONHCH}_3$ and $\text{CH}_3\text{COCH}_2\text{NHCH}_3$

(iii) PhCOOCH_3 and CH_3COOPh

(15 Marks)

- a. (i) Explain the basic principle of a mass spectrometer.
(ii) State four parts of a mass spectrometer.
 - b. (i) Write the structure of 2-methylpentane.
(ii) Give a simplified mass spectrum of 2-methylpentane showing how the chain can break in several places and the most abundant ion. (Hint: Show Relative Abundance for only the base peak)
- (15 Marks)
6. a. Discuss organic pollutants under the following headings:
- (i) Definition
 - (ii) Name of organic pollutant of plant origin and another of animal origin and their sources.
 - (iii) The mode of action and structure of each of the pollutants named in 1a (ii) above.
- b. Give five essential features of spectrometers used for UV/VIS, IR, and NMR techniques.
- c. List two types of radiation absorbed by a molecule. For each, state the effect of the absorption and the information obtainable.
- d. A solution containing 1.0 mol L^{-1} of the solute gave an absorbance of 1.5 when measured in a 1 cm cell. Calculate its molar absorptivity (ϵ).
- (15 Marks)