18

RAJARATA UNIVERSITY OF SRI LANKA

FACULTY OF APPLIED SCIENCES

B.Sc. in Applied Sciences

Second Year – Semester II Examination – September / October 2020

CHE - 2106 SPECTROSCOPIC METHODS IN ORGANIC CHEMISTRY

Time: One (01) hour

Answer all Questions

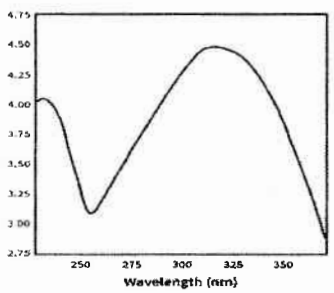
1.

a). A flask of cyclohexane is known to be contaminated with benzene. At 260 nm, benzene has a molar absorptivity of 230 mol^{-1} L m^{-1} and cyclohexane has a molar absorptivity of zero. A UV spectrum of the contaminated cyclohexane (1.0 cm cell length) shows an absorbance of 0.030.

i. What is the concentration of benzene? (5 marks)

ii. What are the limitations of the above absorption method. (5 marks)

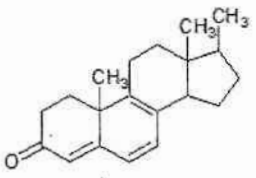
b). Given below the UV spectrum of 3-butene-2-one shows UV absorption maxima at λ_{max} 219 nm and 324 nm. Discuss the electronic transitions of the compound.



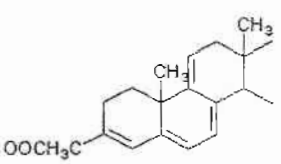
(5 marks)

c). Calculate the UV λ_{max} of the following structures using Woodward-Fischer rule. (Basic value for acyclic conjugated system: 217 nm, acyclic conjugated enone: 215 nm, heteroannular conjugated system: 214 nm, homoannular conjugated system 253 nm, -OR group: 6 nm, homoannulardiene component: 39 nm, extended conjugation: 30 nm, Alkyl substitution: 5 nm, ring residue: 5 nm, Exocyclic double bond: 5 nm, -OAc substitution: 0 nm, α-substitution: 10 nm, β-substitution: 12 nm, γ or higher substitution: 18 nm)

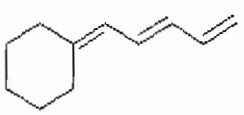
(15 marks)



i.



ii.



iii.

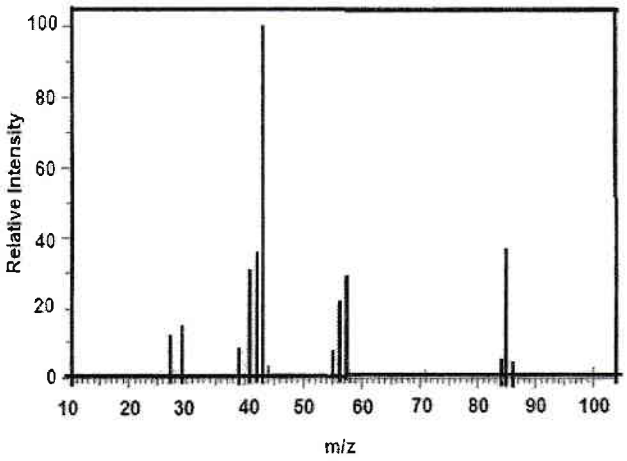
2. a). Write a brief account on electron impact ionization mode of mass spectrometry.

(10 marks)

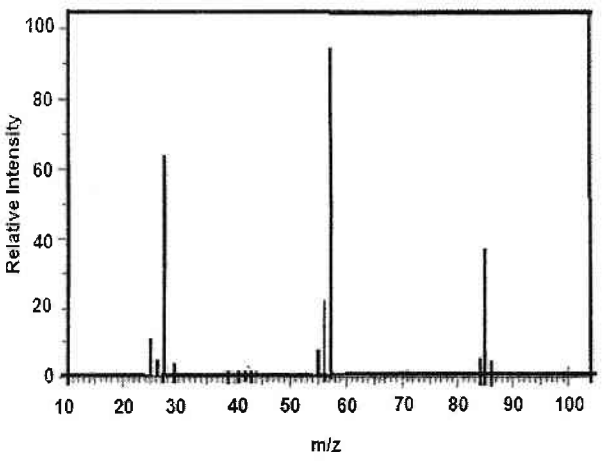
(b). Mass spectrum of 2-methylhexane and 3-pentanone are given below. Identify the relevant spectra and discuss the fragmentation.

(15 marks)

(A)



(B)



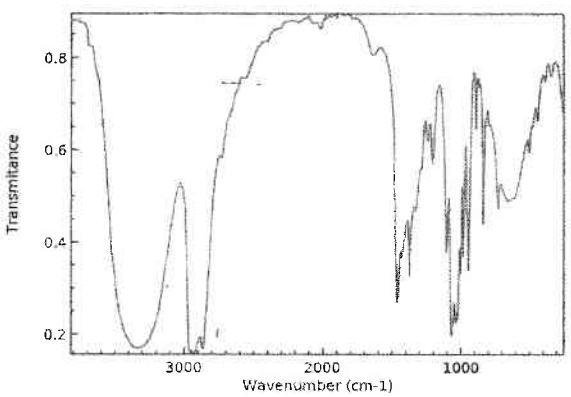
3. (a). Write a short note on the molecular vibrations of a methylene group that give rise to bands in IR spectra.

(10 marks)

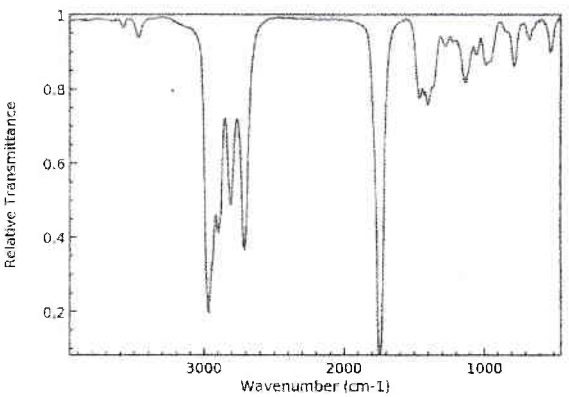
(b). IR spectra of $C_4H_{10}O$ and C_4H_8O are given below. Draw possible structures of the two compounds.

(10 marks)

(A)



(B)

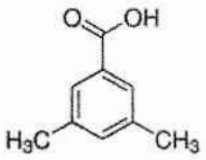


(c). Sketch the high resolution H-NMR of the following compounds.

(15 marks)

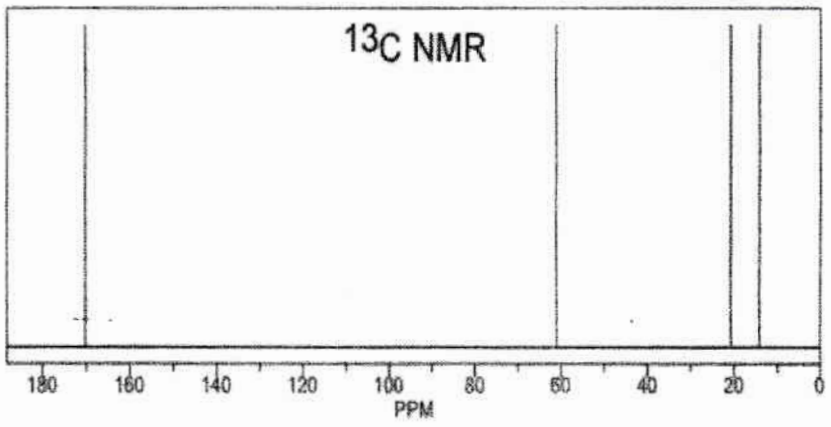
i. $Cl\text{-}CH_2CH_2CH_2\text{-}Cl$

ii. 2,2-dimethylpropanal

iii. 

(d). The 13C-NMR of a compound with molecular formula $C_4H_8O_2$ is given below. Explain the spectrum and suggest a likely structure/s for the compound.

(10 marks)



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