MURANG'A UNIVERSITY OF TECHNOLOGY

SCHOOL OF PURE AND APPLIED SCIENCES

DEPARTMENT OF PHYSICAL AND BIOLOGICAL SCIENCES

UNIVERSITY ORDINARY EXAMINATION

2018/2019 ACADEMIC YEAR

FIRSTYEAR **SECOND** SEMESTER EXAMINATION FORMASTER OF SCIENCE IN CHEMISTRY

ACH 606 – INSTRUMENTAL METHODS OF ANALYSIS

DURATION:3 HOURS

DATE: 23/4/2019

TIME: 2-4 P.M.

Instructions to candidates:

1. Answer **ANY FOUR** questions.
2. Mobile phones are not allowed in the examination room.
3. You are not allowed to write on this examination question paper.

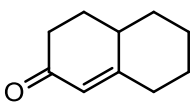
QUESTION ONE (25 MARKS)

a) Distinguish between the following terms. Give examples in each case. (8 marks)

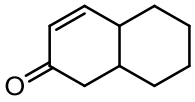
i. Bathochromic shift and hyperchromic shift

ii. Auxochrome and chromophore

b) Explain how UV/visible spectroscopy might be used to distinguish the following compounds (4 marks)

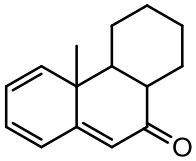


and

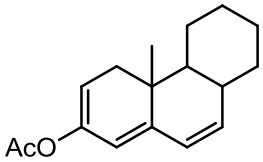


c) Calculate the UV maximum (λ_{max}) for the following molecules (5 marks)

(i)



(ii)



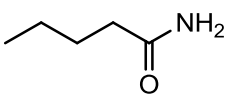
d) Explain how IR spectroscopy might be used to distinguish the following pairs of compounds (8 marks)

i. 1-Hexene and 2,3-dimethyl-2-butene

ii. 1-butanol and butanoic acid

iii. 2-Heptanone and heptanal

iv



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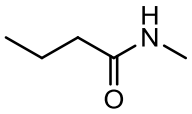
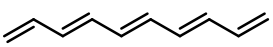


QUESTION TWO (25 MARKS)

a) Account for the observed UV absorption wavelengths in the following molecules (3 marks)

217 nm



334 nm

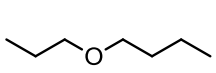
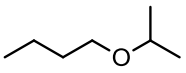
b) Suggest the peaks that might be observed in the mass spectra of the following compounds. For each peak, identify the fragment and suggest a mechanism for the fragmentation. (8 marks)

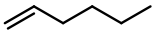
i. 3-Pentanol

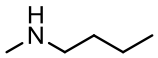
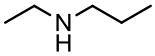
ii. Butylbenzene

c) Explain how the following isomeric molecules might be distinguished using mass spectroscopy. Suggest fragmentation patterns and m/z values of the fragments.

(9 marks)

(i)  and 

(ii)  and 

(iii)  and 

d) The following are the IR and mass spectrum of unknown compound. Propose two possible structures for the unknown compound. Explain. (5 marks)

QUESTION THREE (25 MARKS)

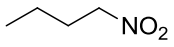
a) Suggest and draw the structures of compounds having the following formulae and given proton spectrum.

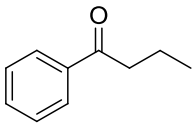
i. $C_5H_{12}O_2$ 4.1(6H, s), 1.8(6H, s) (4 marks)

ii. $C_5H_{10}O$ 5.95(1H,dd,*J*16.5, 7.6), 5.1(dd, 1H, *J*16.5, 1.5), 4.95(1H, dd, *J*16.5, 1.5), 2.2(1H, s, broad), 1.2(6H, s) (4 marks)

iii. $C_6H_{12}O_2$ 3.85(2H, d, *J*7.2), 2.0(3H,s), 1.92(nonet, *J*7.2), 0.9(6H, d, *J*7.2) (4 marks)

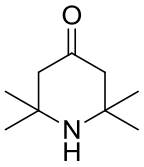
b) Assign the ^1H NMR spectra of these compounds and explain the multiplicity of the signal

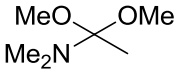
i.)  O.97(3H, t, *J*7Hz), 1.42(2H,Sextet, *J*7Hz), 2.00(2H, quintet, *J*7Hz), 4.40(2H, t, *J*7Hz) (4 marks)

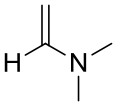
ii.)  1.00(3H,t, *J*7Hz), 1.75(2H, sextet, *J*7Hz), 2.91(2H,t,*J*7Hz), 7.4-7.91(5H, m) (4 marks)

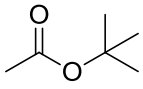
c) Study the following organic moleculesstructures and suggest how many signals will be in their proton NMR spectrum. (5 marks)

i.) 

ii.) 

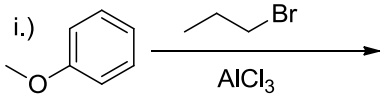
iii.) 

iv.) 

v.) 

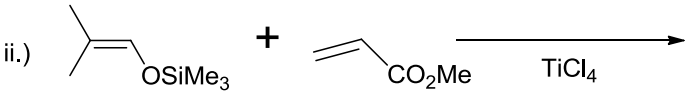
QUESTION FOUR (25 MARKS)

a) Suggest structures for the products of these reactions from interpreting the spectroscopic data provided.

i.) 

Product = $C_{10}H_{14}O$
^{13}C NMR=153, 141, 127, 115, 59, 33, 24
^{1}H NMR= 1.21(6H, d, *J*7Hz), 2.8(1H,Septuplet, *J*7Hz), 3.72(3H, s), 6.74(2H, d, *J*9Hz), 7.18(2H, d, *J*9Hz)

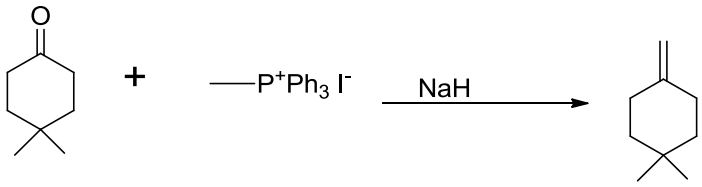
(5 marks)

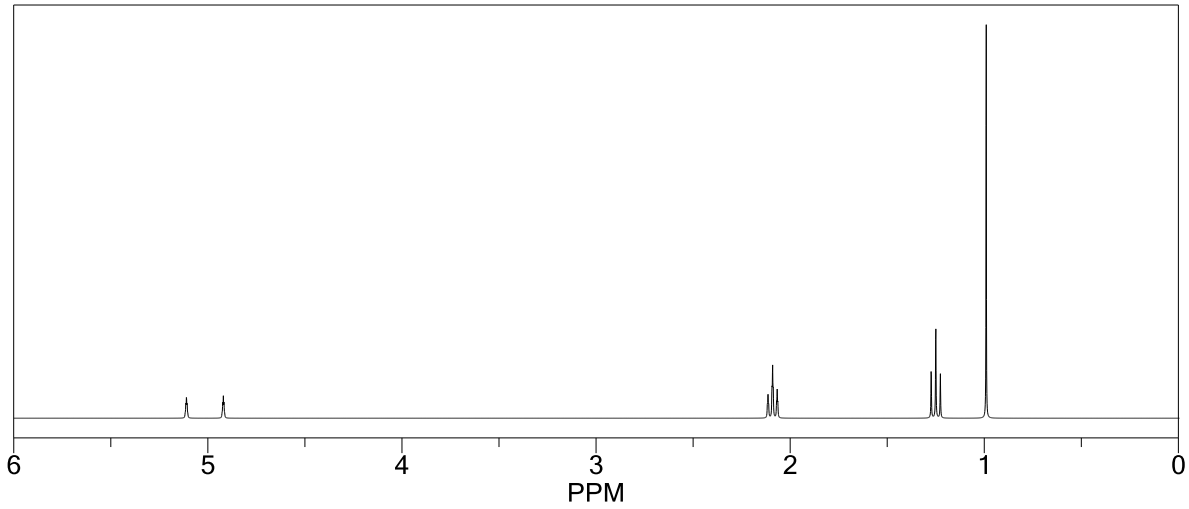
ii.) 

Product=$C_8H_{14}O_3$
^{13}C NMR= 202,176,62,48,34,22,15
^{1}H NMR = 1.21(6H,s), 1.8(2H, t, *J* 7Hz), 2.24(2H, t, J 7Hz), 4.3(3H, s), 10.01(1H, s)

(5 marks)

b) The following Witting reaction between a phosphorium salt, base and an aldehyde gives a hydrocarbon with the 200 MH_z ^{1}H NMR spectrum shown below.





Explain coupling and multiplicity of the signal (9 marks)

c) Briefly explain the following types of coupling

i. Vicinal coupling (2 marks)

ii. Germinal coupling (2 marks)

iii. W-coupling (2 marks)

QUESTION FIVE (25 MARKS)

a) Draw a schematic representation of the atomic absorption spectrometer and explain how the equipment operates. (8 marks)

b) Using Beer's law explain how atomic absorption is used for quantitative analysis. (5 marks)

c) State the three requirements for generation of x-rays in XRD. (3 marks)

d) Write the Bragg equation. (2 marks)

e) List five applications of XRD. (5 marks)

f) Identify two limitations of XRD in analysis. (2 marks)