

**UNIVERSITY OF SWAZILAND  
FINAL EXAMINATION 2017/2018**

---

**TITLE OF PAPER** : ORGANIC SPECTROSCOPY &  
STRUCTURE ELUCIDATION

**COURSE NUMBER** : CHE331

**TIME** : Three Hours

**INSTRUCTIONS** : Answer any **FOUR Questions**. Each  
Question carries 25 Marks.

---

**This Paper contains 14 printed pages.**

***You must not open this paper until the Chief Invigilator so has granted permission to do.***

### Question 1

(a) Define the following terms;

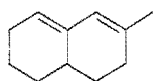
- (i) Spectroscopy
- (ii) Auxochrome
- (iii) Bathochromic Shift
- (iv) Index of hydrogen deficiency
- (v) Fingerprint region

[5]

(b) Explain the differences in  $\lambda_{\max}$  in cisoid and transoid UV absorptions.

[3]

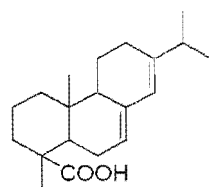
(c) A diene  $C_{11}H_{16}$  was thought to have the structure below. Its UV spectrum showed a  $\lambda_{\max}$  of 263 nm. Can the structure below be correct? If not, draw the structure with the same skeleton that satisfies the spectral data



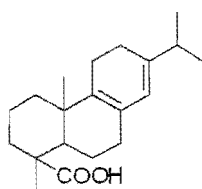
[3]

(d) Can you distinguish between the following three isomeric acids by UV spectroscopy? Use the Woodward-Fieser rules to predict each  $\lambda_{\max}$ .

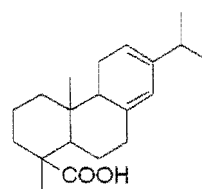
[6]



A



B



C

(e) Propose a structure for an alcohol  $C_4H_{10}O$  that has the following;

$^{13}C$  NMR Spectral data:

Broadband-decoupled  $^{13}C$  NMR: 19.0, 31.7, 69.5  $\delta$

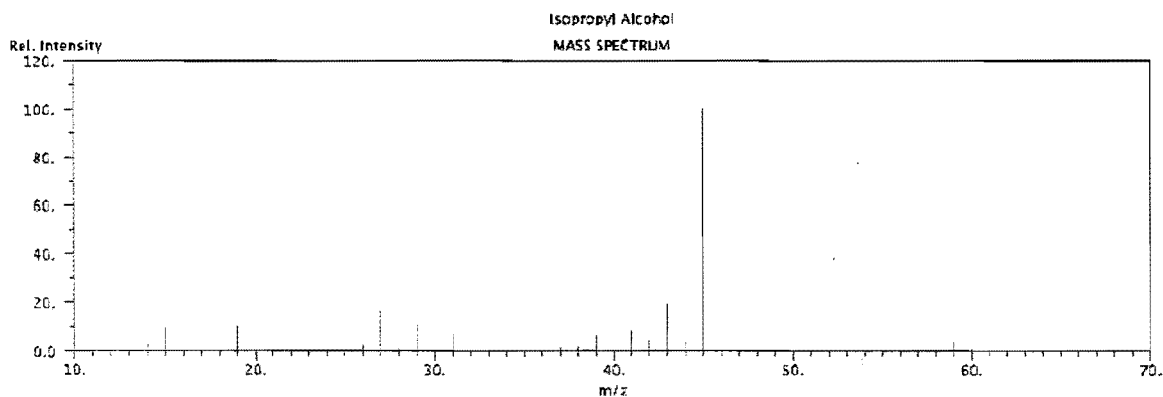
DEPT-90: 31.7  $\delta$

DEPT-135: positive peak at 19.0  $\delta$ , 31.7  $\delta$ , negative peak at 69.5  $\delta$

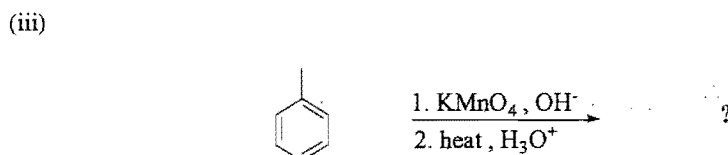
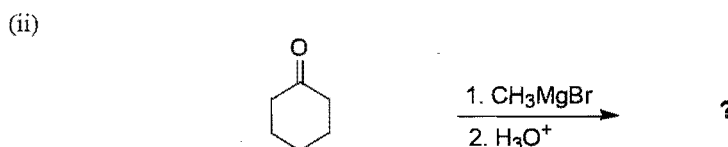
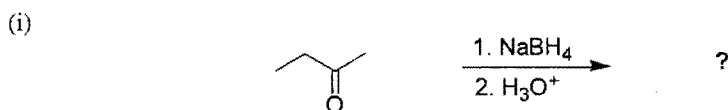
[8]

## Question 2

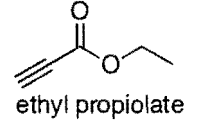
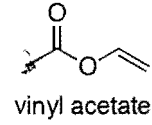
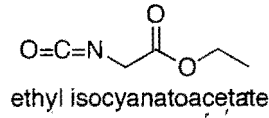
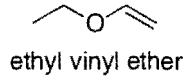
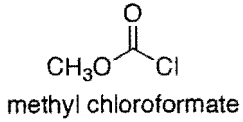
- (a) The electron impact ionization (EI) mass spectrum for 2-propanol is shown below. Write Lewis structures for the species that give rise to the peaks at  $m/z$  45 and  $m/z$  43. Make sure to show all carbon, hydrogen, and oxygen atoms and all bonds, charges, lone pairs of electrons, and unpaired electrons. [6]



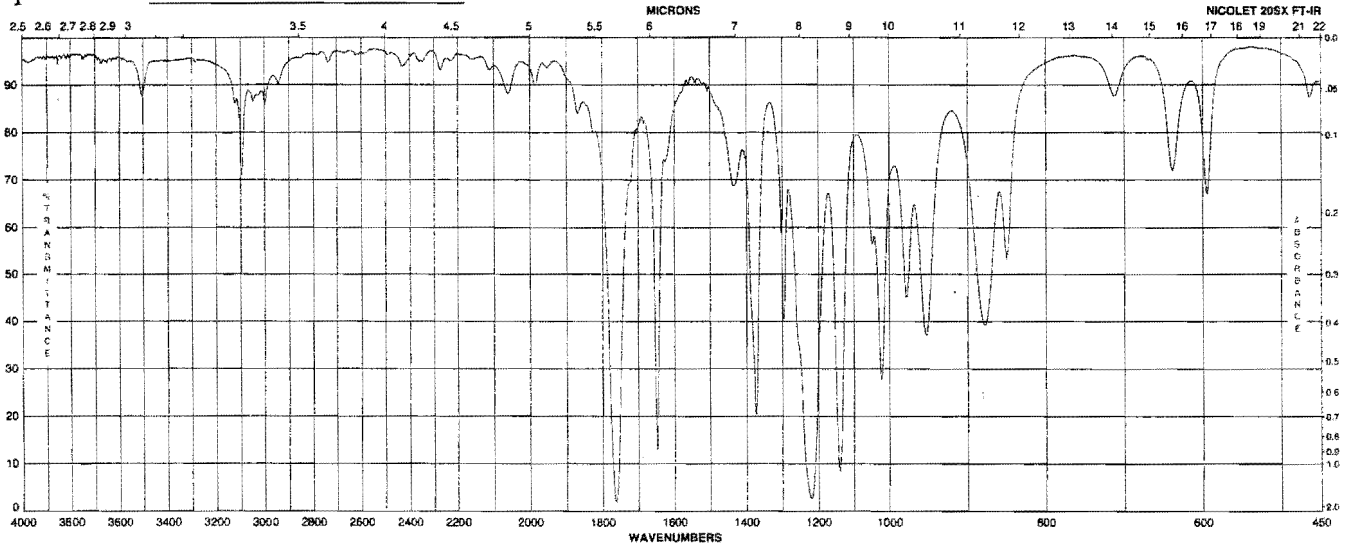
- (b) Write the products of the following reactions. Propose plausible IR absorption bands and  $m/z$  of the products.



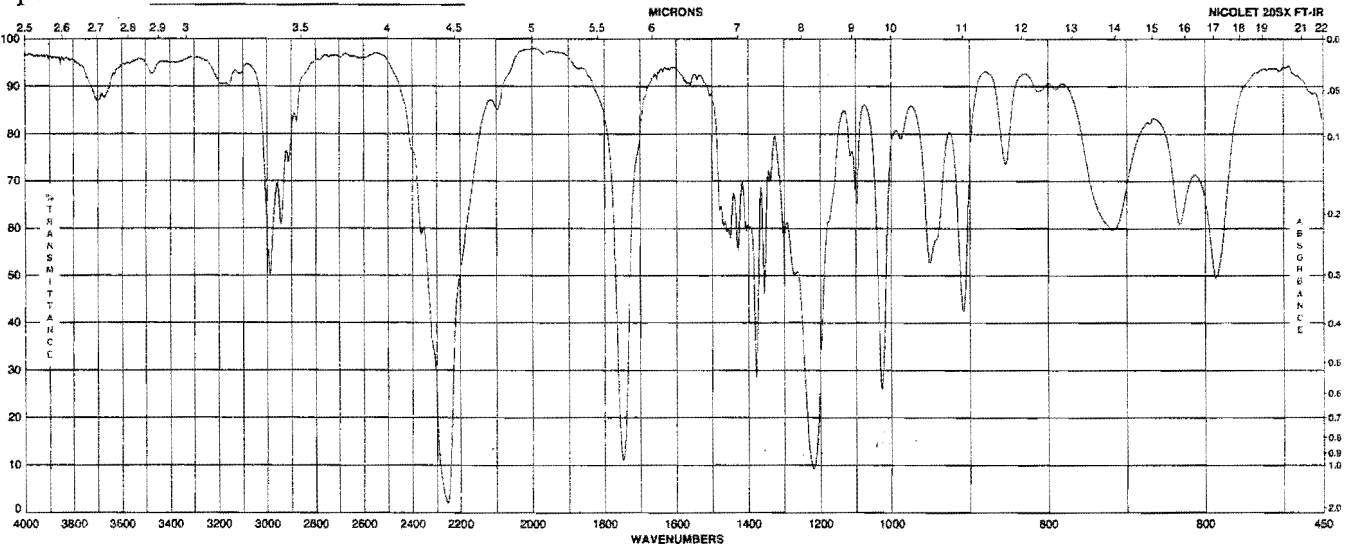
(c) Each of the following IR spectra is associated with one of the compounds below. Identify the compound associated with each spectrum. [10]



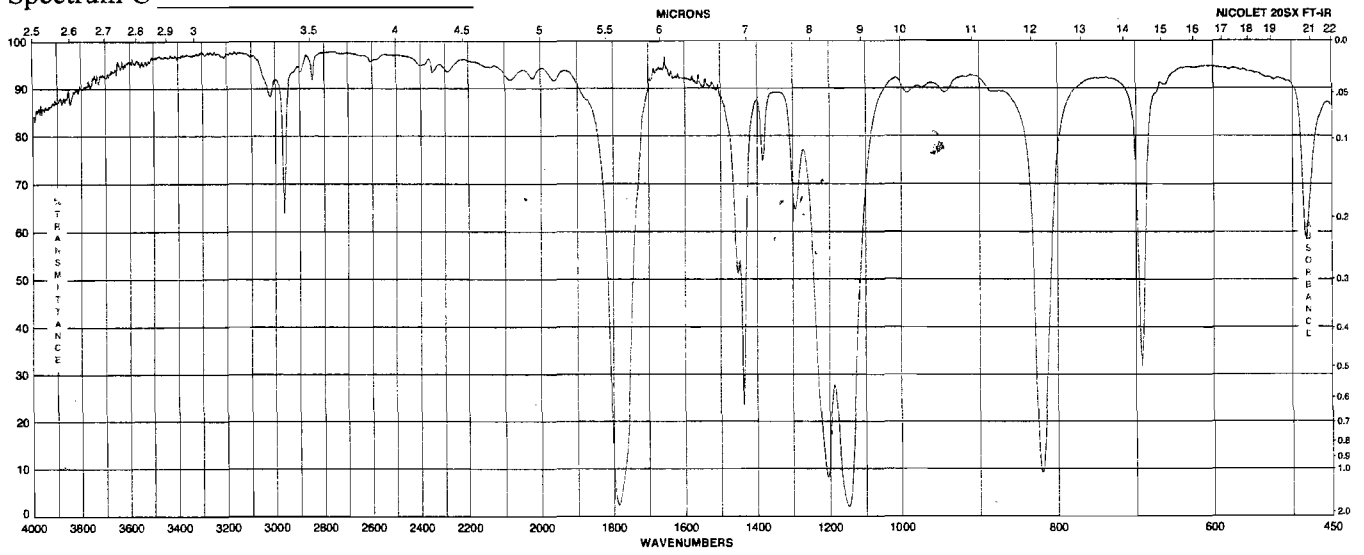
Spectrum A



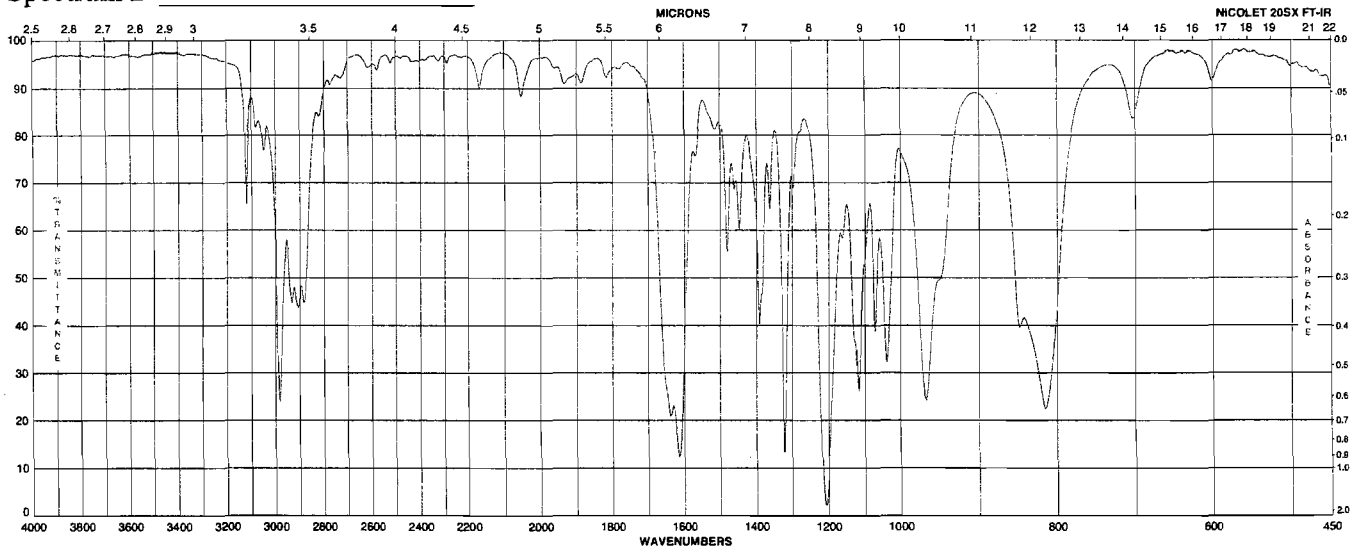
Spectrum B



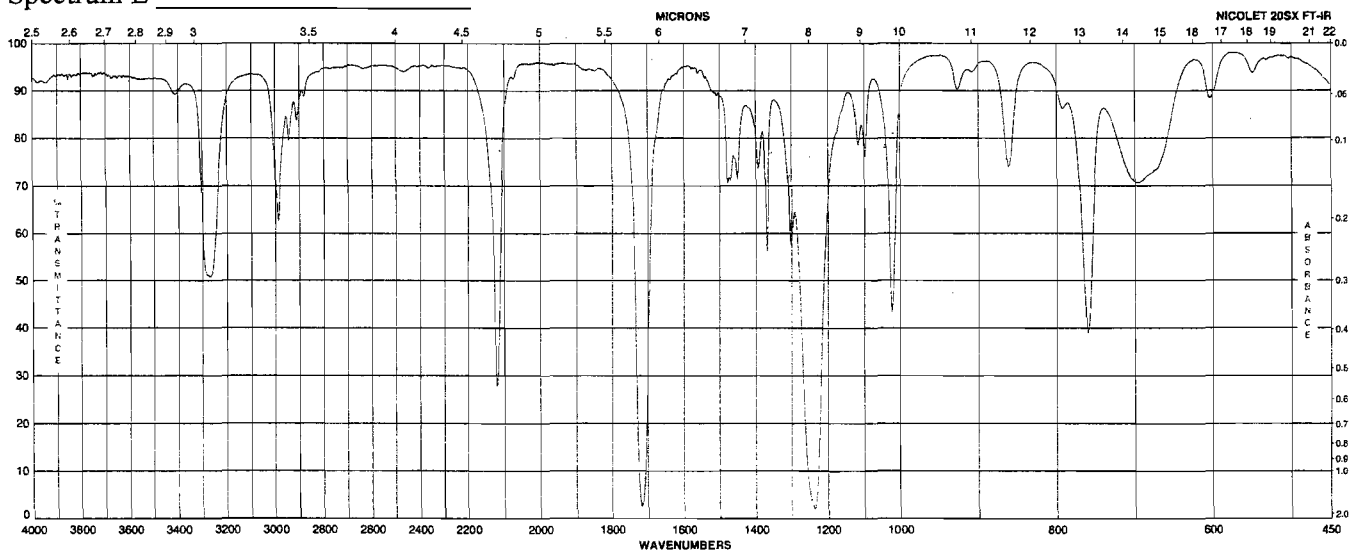
Spectrum C



Spectrum D



Spectrum E



### Question 3

- (a) The integrated  $^1\text{H}$ NMR spectrum of a compound of formula  $\text{C}_4\text{H}_{10}\text{O}$  is shown below. Examine the spectrum, interpret all signals and propose a structure. [8]

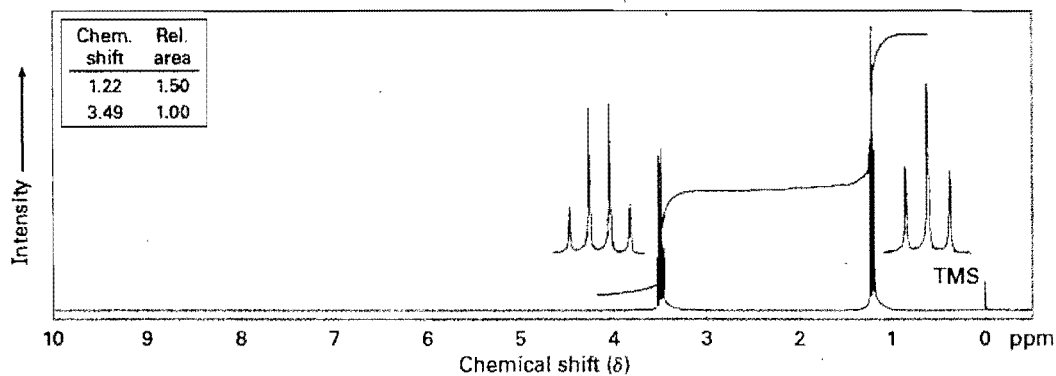


Figure X; The Intergrated  $^1\text{H}$ NMR Spectrum of  $\text{C}_4\text{H}_{10}\text{O}$

- (b) Propose a structure for an aromatic hydrocarbon,  $\text{C}_{11}\text{H}_{16}$ , that has the following  $^{13}\text{C}$  NMR spectral data:  
 Broadband decoupled: 29.5, 31.8, 50.2, 125.5, 127.5, 130.3, 139.8  $\delta$   
 DEPT-90: 125.5, 127.5, 130.3  $\delta$   
 DEPT-135: positive peaks at 29.5, 125.5, 127.5, 130.3  $\delta$ ; negative peak at 50.2  $\delta$  [9]
- (c) Compound A,  $\text{C}_4\text{H}_8\text{O}_3$ , has infrared absorptions at 1710 and 2500 to 3100  $\text{cm}^{-1}$  and has the  $^1\text{H}$  NMR spectrum shown below. Propose a structure for A. [8]

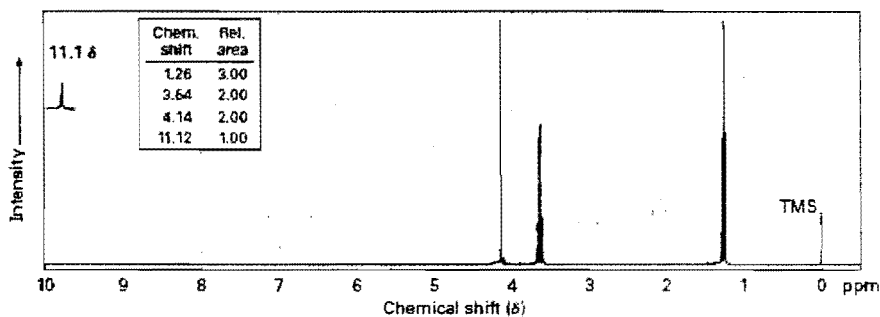


Figure X;  $^1\text{H}$  NMR spectrum of  $\text{C}_4\text{H}_8\text{O}_3$

### Question 4

- (a) Determine the molecular formula and draw possible structures for each unknown based on the given spectra. Also, calculate the index of hydrogen deficiency for each structure. All mass spectra are CI. SHOW YOUR WORK!

(i)

