21.1 Spectroscopic Identification of Organic compounds

Question Paper

Course	DP IB Chemistry
Section	21. Measurement & Analysis (HL only)
Topic	21.1 Spectroscopic Identification of Organic compounds
Difficulty	Easy

Time allowed: 60

Score: /43

Percentage: /100

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Question 1a

a)
Three important analytical techniques in the chemist's toolkit are Mass Spectrometry, MS, Infrared Spectroscopy, IR and Nuclear Magnetic Resonance Spectroscopy, NMR.
For each technique identify the characteristic chemical information provided.

[3]

[3 marks]

Question 1b

b)
For each of the following, identify their significance in an ^{1}H NMR spectrum: number of peaks, area under each peak, chemical shift and splitting patterns.

[4]

[4 marks]

Question 1c

c)
^{1}H NMR spectroscopy uses tetramethylsilane. State its formula and purpose in ^{1}H NMR spectroscopy.

[2]

[2 marks]

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Question 1d

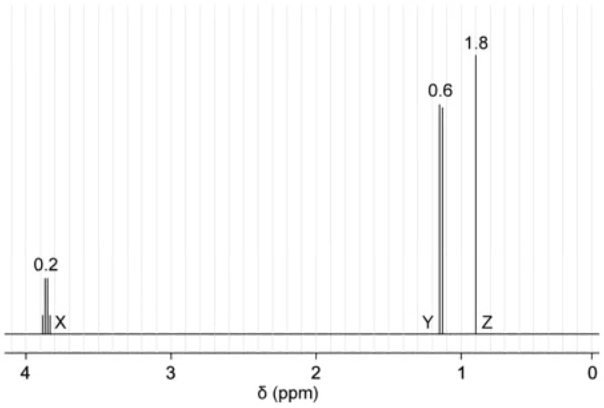
d)
State three advantages of using TMS in an ^{1}H NMR spectrum.

[3]

[3 marks]

Question 2a

a)
Part of the ^{1}H NMR spectrum of an organic compound is shown below:



Determine the number of unique hydrogen environments

[1]

[1 mark]

Question 2b

b)
Deduce the whole number ratio of the hydrogen environments in the spectrum.

[1]

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[1 mark]

Question 2c

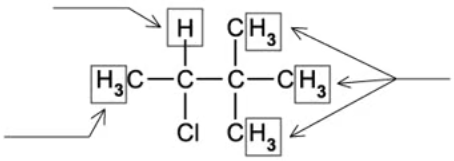
c)
State the splitting patterns present in the spectrum and suggest what information could be obtained from the patterns.

[4]

[4 marks]

Question 2d

d)
Assign peaks X, Y and Z to the correct location shown in the compound:



[2]

[2 marks]

Question 3a

a)
Outline what chemical information can be obtained about inorganic ionic substances and complex organic molecules from X-ray crystallography studies.

[2]

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[2 marks]

Question 3b

b)
Explain why X-ray crystallography is not very useful for compounds containing hydrogen.

[2]

[2 marks]

Question 3c

c)
Suggest another limitation of X-ray crystallography for organic compounds.

[1]

[1 mark]

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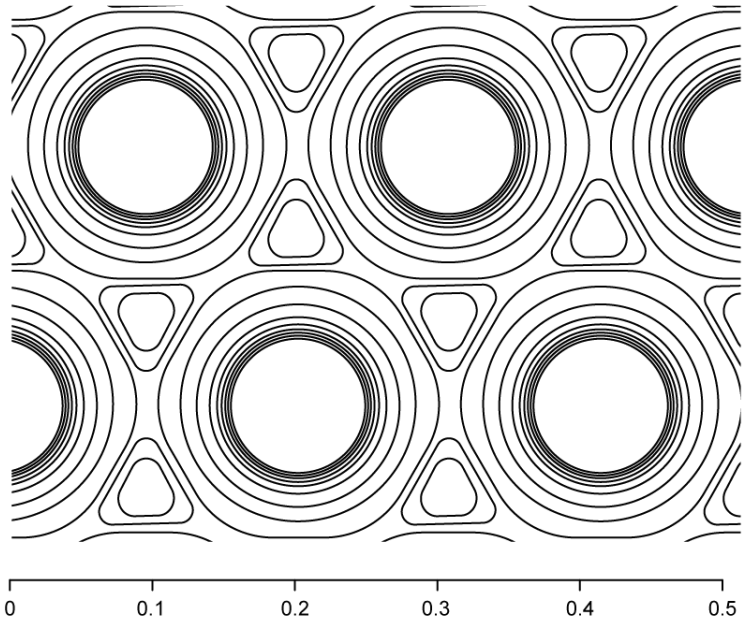
Question 3d

d)

An electron density map obtain from the X-ray crystallography of copper metal is shown below:



Use the diagram to estimate the radius of a copper atom. The units are nm.

[1]

[1 mark]

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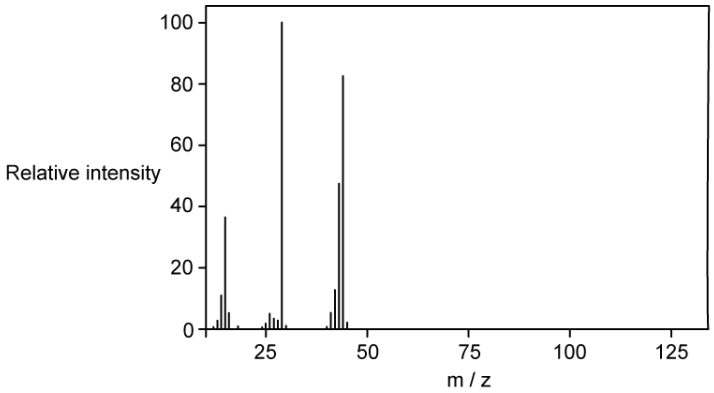
Question 4a

a)

An organic molecule with molecular formula C_2H_4O is analysed using MS, IR and ^1H NMR. Use section 26, 27 & 28 of the Data booklet to help you answer this question.

The MS is shown below:



Determine the relative molecular mass from the spectrum and account for the peak at m/z 29.

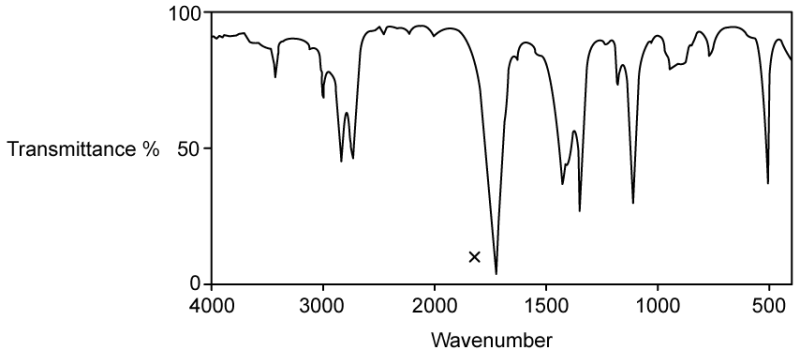
[2]

[2 marks]

Question 4b

b)

The IR spectrum of the same compound is shown below.



Identify the functional group responsible for the peak at X

[1]

[1 mark]

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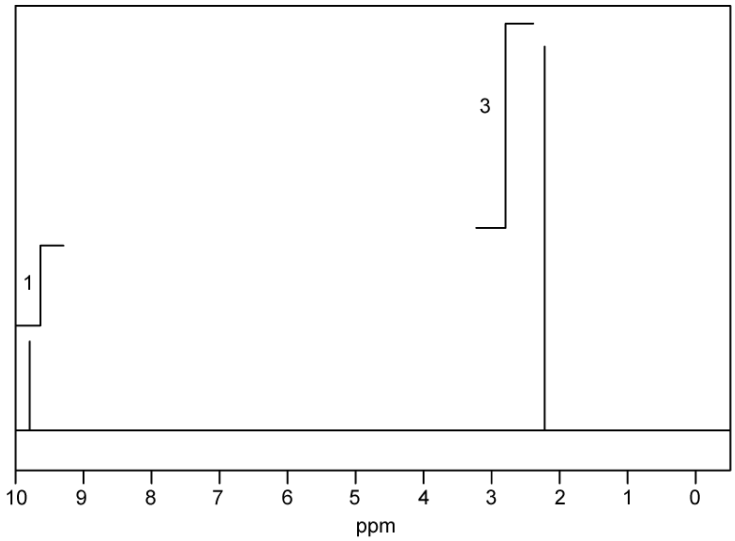
Question 4c

c)
The ^{1}NMR spectrum of C_2H_4O is shown below:



Account for the peaks at 2.2 ppm and 9.8 ppm and their relative areas.

[3]

[3 marks]

Question 4d

d)
Deduce the displayed structure of this compound from the spectroscopic information.

[1]

[1 mark]

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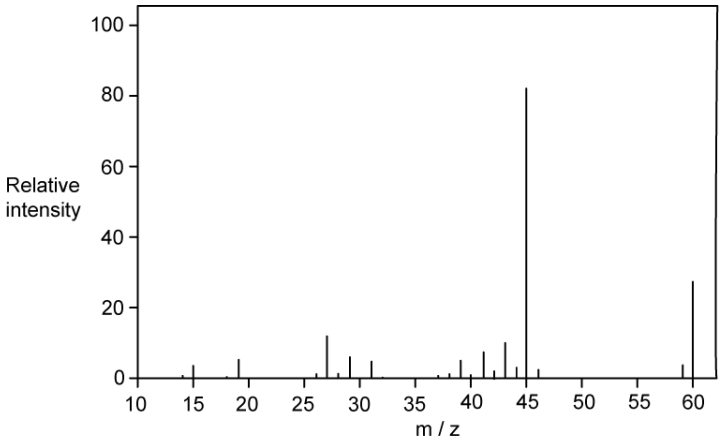
Question 5a

a)

The MS of compound P is shown below. Compound P contains carbon, hydrogen and oxygen only. Use section 26, 27 & 28 of the Data booklet to help you answer this question.



Determine the relative formula mass of P and account for the peak at m/z 45.

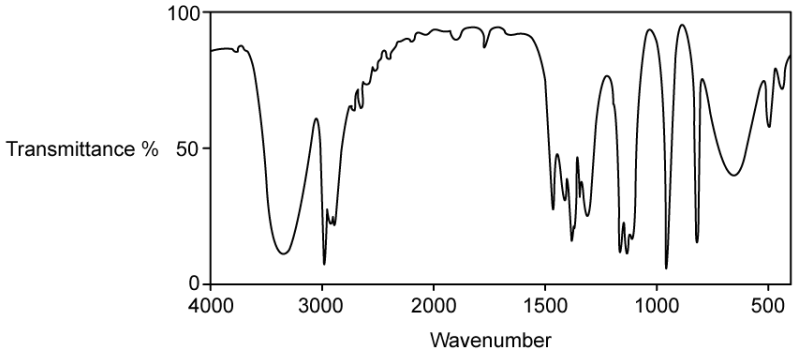
[2]

[2 marks]

Question 5b

b)

The IR spectrum of P is shown below.



Use the spectrum and your answer to part a) to deduce a functional group that could be present in P.

[2]

[2 marks]

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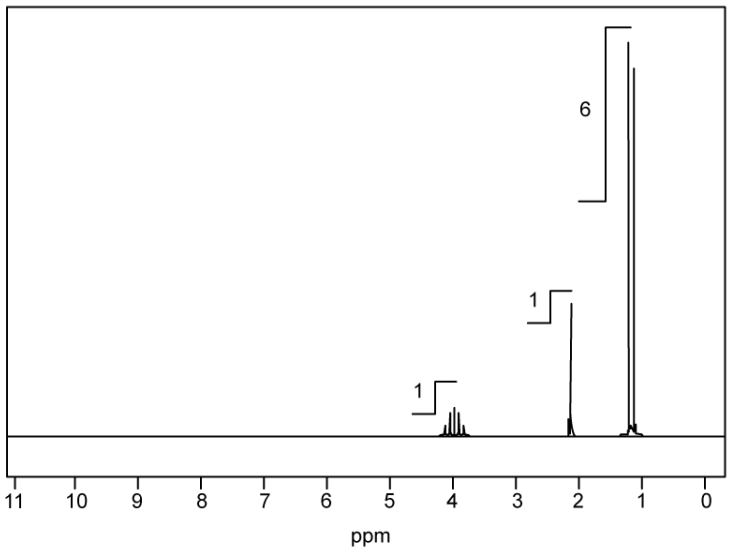
Question 5c

c)
The 1H NMR spectrum of P is shown below.



Deduce what information can be found from the spectrum.

[2]

[2 marks]

Question 5d

d)
A student suggests that P is propan-1–ol. Evaluate all the evidence from the spectra and determine whether the student is correct.

[4]

[4 marks]

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