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	Hard

Time allowed: 50

Score: /40

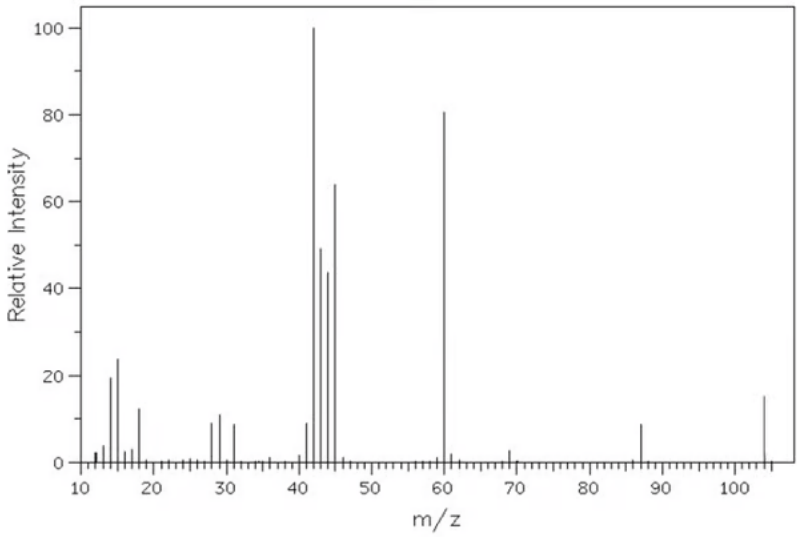
Percentage: /100

Question 1a

a)

Malonic acid, $C_3H_4O_4$, is naturally occurring and found in many fruits and vegetables. It contains only carbon, hydrogen and oxygen.

The MS of malonic acid is show below.



Determine the relative molecular mass of malonic acid from the spectrum and account for the peak at m/z 45, using section 28 of the Data booklet to support your answer.

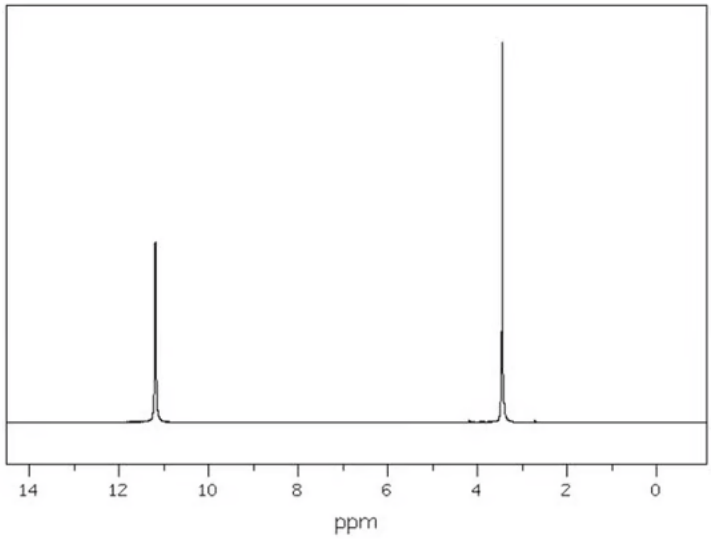
[2]

[2 marks]

Question 1b

b)

The ^{1}H NMR spectrum of malonic acid is shown below. Use section 27 of the Data booklet to help you with this question.



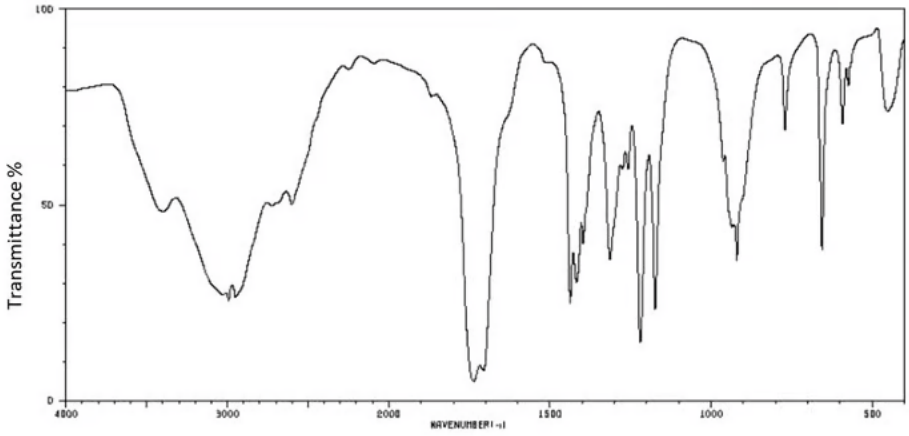
Suggest the identity of the proton environments seen in the spectrum and comment on the type of signals shown.

[3]

[3 marks]

Question 1c

c)
The IR spectrum of malonic acid is shown below:



i)
Identify two characteristic peaks and bonds that can be found in the spectrum of malonic acid.

[2]

ii)
Explain how the spectrum can be used to distinguish malonic acid from ethanoic acid.

[1]

[3 marks]

Question 1d

d)
Draw a displayed structure for malonic acid.

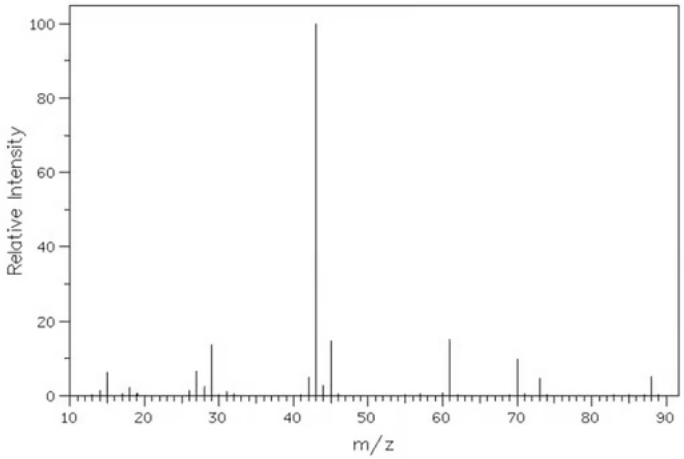
[1]

[1 mark]

Question 2a

a)

An organic compound, Q, of molecular formula $C_xH_yO_z$, has the following MS. Use section 28 of the Data booklet to help you answer this question.



i)

Determine the relative molecular mass of Q and account for the peaks at 15 and 29.

[2]

ii)

Comment on the size of the peak at m/z 43.

[1]

iii)

Write an equation for the formation of the fragment at m/z 29.

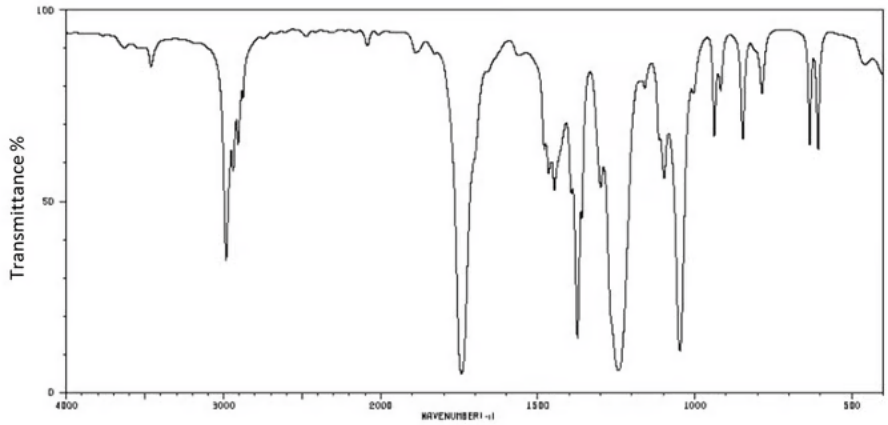
[1]

[4 marks]

Question 2b

b)

The IR spectrum of Q is shown below.



Suggest which functional group(s) could be present in Q.

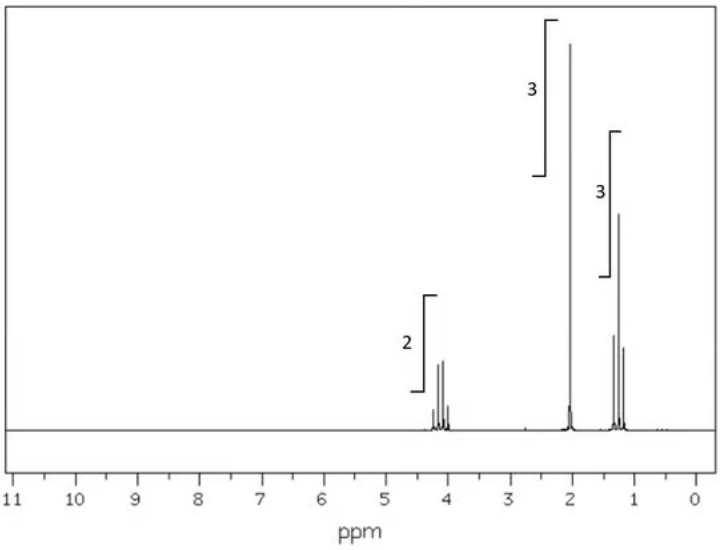
[1]

[1 mark]

Question 2c

c)

The ^{1}H NMR spectrum of Q is shown below.



Explain the relative peaks heights and splitting patterns

[5]

[5 marks]

Question 2d

d)
Suggest the identity of Q, giving your reasons.

[3]

[3 marks]

Question 3a

a)

Compound A, has molecular formula C_5H_{10} and occurs as 6 isomers. The table below shows the number of signals in the NMR spectrum of each isomer.

Isomer	Number of ^1H NMR signals
A	1
B	5
C	5
D	5
E	5
F	4

Suggest a structure for A and F.

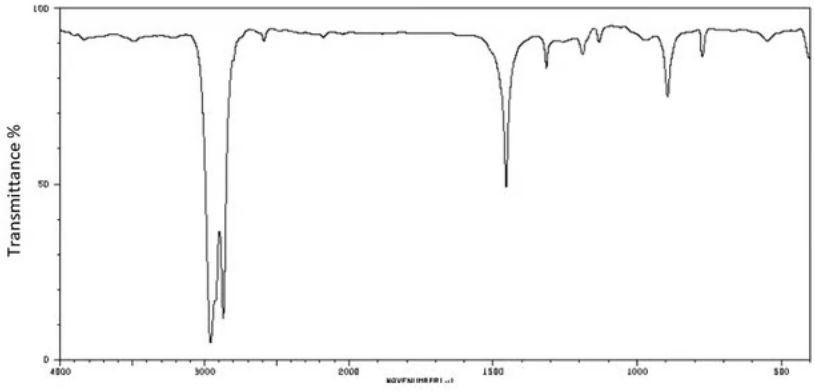
[2]

[2 marks]

Question 3b

b)

The IR spectrum of A is shown below.



How does this spectrum distinguish A from the other isomers?

[3]

[3 marks]

Question 3c

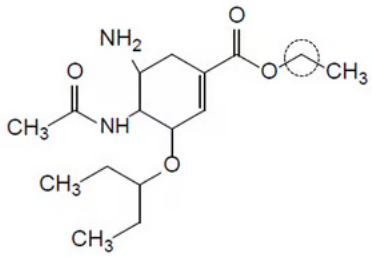
c)
Evaluate whether X-ray crystallography could distinguish between the isomers of A.

[1]

[1 mark]

Question 4a

a)
Oseltamivir is a drug used to treat and prevent influenza A and influenza B.



Predict the number of different proton environments in the molecule.

[1]

[1 mark]

Question 4b

b)
Predict the chemical shift and the splitting pattern seen for the hydrogens on the carbon atom circled in the diagram. Use section 27 of the Data booklet.

[2]

[2 marks]

Question 4c

c)
Predict three absorptions you would expect to see in the IR spectrum of oseltamivir. Use section 26 of the data booklet.

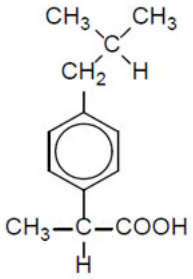
[3]

[3 marks]

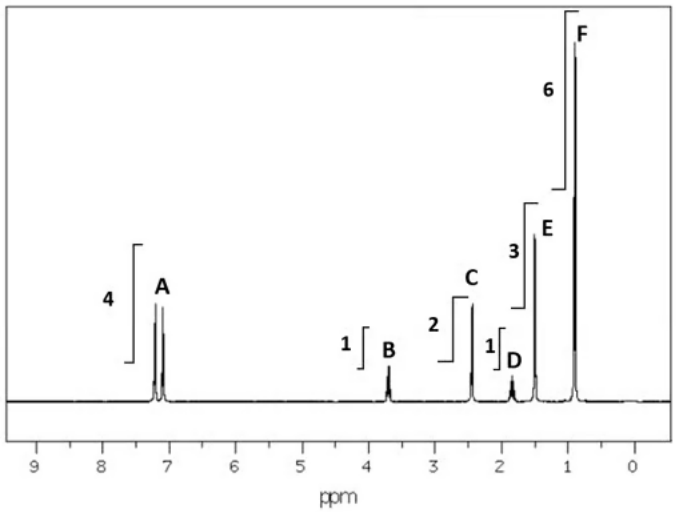
Question 5a

a)

Ibuprofen is an important painkilling drug. The structure is:

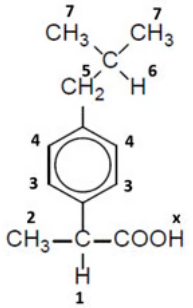


Part of the low resolution ^{1}H NMR spectrum is shown below.



The high resolution expansion of the peaks in B-F is:

The protons responsible for the peaks are numbered 1–7:



Complete the table to show the assignment of the missing peaks.

Peak	H atoms responsible
A	3 & 4

B	
C	
D	
E	
F	
off spectrum	X

[3 marks]

Question 5b

b)
A sample of ibuprofen shows strong absorptions at 1716 cm^{-1} and 3345 cm^{-1} in an IR spectrum. Suggest the bonds responsible for these absorptions using section 26 of the data booklet.

[2]

[2 marks]

Question 5c

c)
A sample of ibuprofen rotates plane polarised light. Identify the feature in ibuprofen responsible for this.

[1]

[1 mark]