National Certificate of Educational Achievement
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Exemplar for Internal Assessment Resource

Chemistry Level 3

Resource title: Solving organic structural problems

This exemplar supports assessment against:

Achievement Standard 91388

Demonstrate understanding of spectroscopic data in chemistry

Student and grade boundary specific exemplar

The material has been gathered from student material specific to an A or B assessment resource.

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	Grade Boundary: Low Excellence
1.	To meet Excellence students need to demonstrate comprehensive understanding of spectroscopic data in chemistry. All techniques (mass, infrared and NMR spectroscopy) have been integrated to identify Compound A. However, the peak at m/z=57 in the mass spec is incorrectly accounted for as due to molar mass **(1)**. No units have been used to interpret the IR spectroscopy for Compound B **(2)**. To meet Excellence more securely it should be stated the peak at m/z=57 is due to the loss of the Br group, and units should be used in interpreting the IR spectroscopy for Compound B.

Student 1: Low Excellence

1.a.

i. 137 mass units is the molar mass of Compound A. The molar mass of Bromine is 80, and the molar mass of C_4H_9 is 57. 80 + 57 = 137, therefore the identity of halogen X is Bromine.

ii. The most likely reason for the peak at 57 is because 57 is the molar mass of C_4H_9. (1)

b.i Isomer 1 has 3 chemical environments, Isomer 2 has 3 chemical environments, Isomer 3 has 2 chemical environments and Isomer 4 has 3 chemical environments.

ii. Isomer 3 matches the structure of compound A because it only has 2 chemical environments and TMS, which is just a reference point.

c. The structural feature responsible for the group of peaks at Y is C-H bonds.

d. The substitution reaction to produce an alcohol has taken place. You can see this because there is a trough present at 3300. This is evidence of O-H bonds being present. Also there is no peaks at 1705-1935, indicating a lack of a carbonyl group which would rule out an alkene.

(2)

	Grade Boundary: High Merit
2.	To meet Merit students need to demonstrate in-depth understanding of spectroscopic data in chemistry. The structure of organic molecules have been justified by integrating spectroscopy data from the different techniques. However, the incorrect molecular formula is given for Compound D **(1)**. In Compound C, the presence of the OH group in butanoic acid and the absence of it in the other molecule are not linked **(2)**. To meet Excellence the correct molecular formula should be stated and there should be linking of the presence of OH in butanoic acid and its absence in the other molecule.

Solving Organic Structural problems

1)

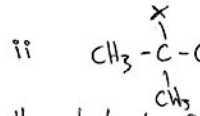
a)

i) The molar mass of the halogen x is Compound A is 137. Does because the halogen labled x is bromine. ~~both~~ we know this because of the 1:1 ~~ratio~~ ratio the compound A is worked out by adding the molar mass of C_4H_9 (57) to bromine 80 57 + 80 = 137.

ii) The most likely reason for the peak at 57 is the bromine is the most easily broken off substance in the molecule. 57 is the molar mass once the bromine is broken off.

b) Isomer

i
~~Product~~ 1 has 3 different possible products
~~Product~~ Isomer 2 has 3 different possible products
Isomer 3 has 2 different possible products
Isomer 4 has 4 different possible products

ii 

c) The structural feature of an organic compound that is responsible for the group of peaks is C-H

D) Since there is a trough at 3200 it is a substitution reaction to produce the Alcohol O-H

2) The molar mass of compound C is around about 86. I know this because on the mass spec graph the highest point is around about 86. This will help us identify compound C ~~because~~ because it will eliminate the other 3 compounds as

2)b) b In the IR spectrum the functional groups that are present in Compound C are the C-H bonds these are represented by the peaks on the graph just below the 3000 mark. another group present is the C=O bond, this shown by the single peak around 1700 - 1750. ~~#~~ Since there is no trough on the graph above 3000, we know that there is not an ~~O-H~~ O-H

2)c) In Compound C there a 3 chemical environments present. The 3 peaks are shown by the 3 peaks on the ^{13}C NMR spectrum. On the spectrum there is another peak ~~#~~ at 75 this is the TMS The peaks show the chemical environments

2) d)

The compound C is Pentan-3-one

In Pentane-3-one there is the functional group C-H and C=O. But no O-H. There is also three chemical environments ($CH_3CH_2C=O$) which was identified in the ^{13}C NMR spectrum. Also the molar mass of the compound matches the one from the spectral data which was 86

3) The molar mass of compound D is 88, this is shown by the small peak that is the furthest away on the right with this ~~info~~ data we know that the molecular formula is C_4H_8O as it has a molar mass of 88 (1)

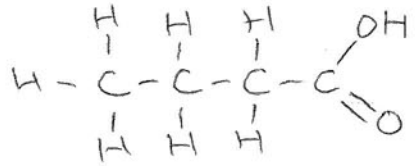
3 b) Using the IR spectrum we can identify the functional groups present in the compound which are O-H which is shown by a trough just above 3000, peaks just below 3000 show C-H bonds. and the peak around 1760 shows us that C=O bonds are there.

	Grade Boundary: Low Merit
3.	To meet Merit students need to demonstrate in-depth understanding of spectroscopic data in chemistry. Mass spectroscopy has been used well to determine the empirical formula **(1)**. IR spectroscopy has also been used. However, not all the possible structures have been identified. NMR data has not been used. To meet Merit more securely NMR data should be used and structures should be identified by using IR data.

3a Compound D has a Mr of 88 g mol^{-1} because the peak furtherest to the right in the Mass spectrum graph is on 88. The molar mass of C_2H_4O is 44 g mol^{-1}. $88 \div 44 = 2$ so the molecular formula will be 2× the empirical formula of C_2H_4O which is $C_4H_8O_2$. (1)

b OH, C=O. The OH is shown by the big drop at about 3000 and the C=O is shown by the sharp point at about 1750. This suggests the functional group is an acid.

c) ?

d 

	Grade Boundary: High Achieved
4.	To meet Achievement students need to demonstrate understanding of spectroscopic data in chemistry. Mass spectroscopy data has been used but there is no link between the molar mass and identification of Compound C **(1)**. From the IR data, the carbonyl group has not been correctly identified **(2)**. NMR data has been used to identify the compound but could have elaborated more by stating how many peaks would be present for the other molecules. To meet Merit there should be an explanation how the molar mass can help identify Compound C and the IR data should be use to correctly identify the carbonyl group and link the presence/absence of peaks to all of the molecules in a systematic way.

Student 4: High Achieved

1a

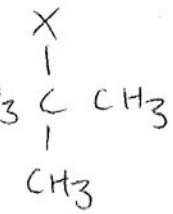
i) Mr = 137-57 = 80
Halogen X = Bromine 1:1 ratio

ii) excess compound from when Bromine experienced ionisation and broken off into fragments

b

i) 3, 3, 2, 3

ii) Product 3. Only one with two carbons



c) C-H

d) ———

2a) Mr of Compound C is 87±1 as it is at the peak furthest to the right. (1)

b) The function groups present in compound C are C-H, C=O. C-H is at 3000 and is a jaggered dip. At 1750 there is one icecle shaped dip and this is C-H (2)

c) Number of chemical enviroments is 3. There are 4 spikes, but one is TMS. This shows that it is pentan-3-one

d) Compound C is pentan-3-one because it has a molar mass of 86 complying with the graph of mass spectrum. The C=O is the big dip on the I.R Spectrum at about 1735. There are 3 chemical enviroments on pentan-3-one, where the others do not have 3.

	Grade Boundary: Low Achieved
5.	To meet Achievement students need to demonstrate understanding of spectroscopic data in chemistry. Some discreet aspects of the spectroscopy data have been identified. In (a), the wrong formula has led to confusion within the answer **(1)**. There is no clarity in the chosen structure for the data as butanone as well as the correct structure has been drawn **(2)**. Also, the OH group has been identified from the shape and not from the numerical value. To meet Achievement more securely mass spectroscopy data should be used more accurately to identify the correct molar formula and the OH group should be identified from the numerical value provided by the IR data.

Student 5: Low Achieved

3) a) The molecular mass of compound D is at around MR 88

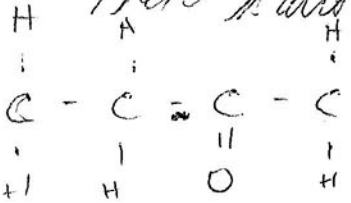
C_2H_4O Ethanal $(12\times2)+(4\times1)+16 = 44$

C_4H_8O Butanal $(12\times4)+(8\times1)+(16\times2) =$ MR 88

Judging by the molecular mass that was given by the mass spectrum, Butanal would likely be compound D. since it has the ~~same~~ same molecular mass of 88 MR that was shown in the mass spectrum. (1)

b) The IR spectrum shows at around 3000 there is a peak that can be identified as a C-H bonding. and at 1700 in the IR spectrum suggest that there is a C=O bonding present on on the peak of the graph. There is also half of a parabola that suggest that there is an O-H bonding

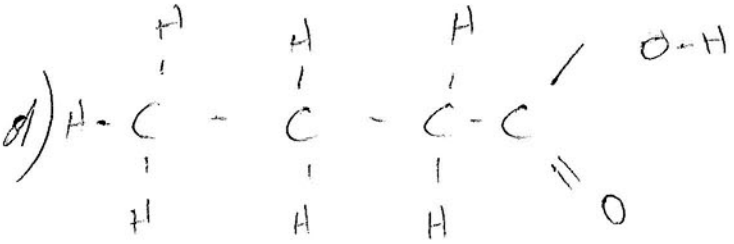
c)



From the ^{13}C NMR spectrum there is 4 different electronic carbon environments that is present in the graph

(2)

d)



Butanoic acid

	Grade Boundary: High Not Achieved
6.	To meet Achievement, students need to demonstrate understanding of spectroscopic data in chemistry. There is an attempt to use mass spectroscopy data as the molecular ion peak has been identified. However, mass spec data has not been used to identify halogen X **(1)**. Also, no structures in (d) have been identified or identified that the peak is due to the OH group which is present in alcohols **(2)**. To meet Achievement, either the halogen X should be identified by using mass spec data or the structures in part (d) should be identified using IR spec data.

Student 6: High Not Achieved

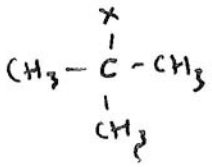
1.

a) i. 138

ii. A butyl group (1)

b) i. 4 , 4 , 2 , 3

ii.



c) C-H bond

d) substitution to form an alcohol as there is a peak after 3000 (2)