National Certificate of Educational Achievement
TAUMATA MĀTAURANGA Ā-MOTU KUA TAEA

Exemplar for Internal Assessment Resource

Chemistry Level 3

Resource title: Identifying the reaction products

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.

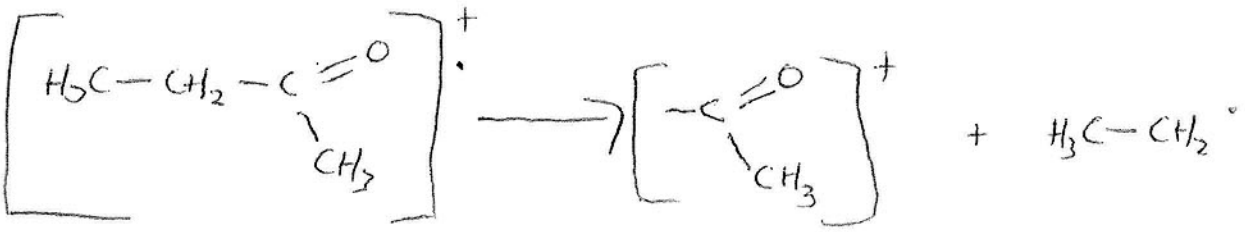
Date version published by Ministry of Education

December 2012
To support internal assessment from 2013

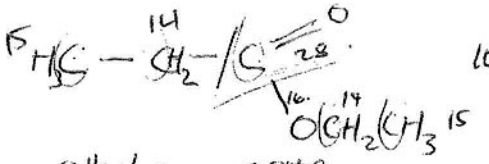
	Grade Boundary: Low Excellence
1.	To meet Excellence students need to demonstrate comprehensive understanding of spectroscopic data in chemistry. The structure of organic molecules have been identified. The structure of organic molecules has been linked to spectroscopic data from different techniques. The structure of these molecules has also been justified by integrating spectroscopic data from different techniques. However, the explanation of molecular ion peak (Tasks a and b) and NMR in Task (c) is not thorough. To meet Excellence more securely a thorough explanation of molecular ion peak and NMR is required.

C=O in the
peak representing the C=O. For Ther ketone, butanone, would be recognised with a peak ~~at~~ in the range of 205-220ppm and in aldehyde, butanal, would be in the range of 190-220ppm. In this case, the peak at approximately 210ppm ~~is~~ clearly represents the C=O present in butanone. Therefore the compound is ketone, butanone.

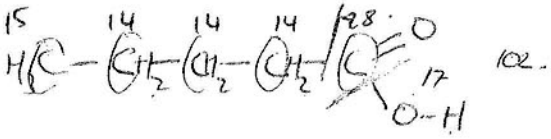
a.(i) Therefore in the mass spectrum, its Mr = 72;
So its base ~~a~~ peak is ~~at~~ ~~43m/z~~ would be at 43m/z.
Base peak = ~~43~~ 43m/z.



b)

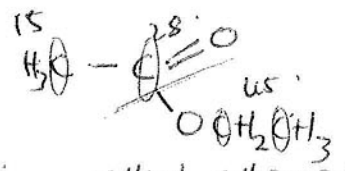


ethyl propanoate.
5 carbon environments.

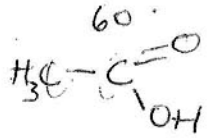


pentanoic acid.
5 carbon environments.

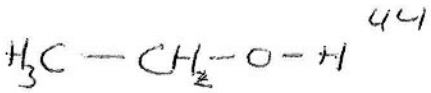
In a ~~MRR~~ NMR Spectrum, each peak would represent a carbon from the different environments. In both ethylpropanoate and pentanoic acid, there are 5 carbon environments, therefore the number of carbon environments would equal the number of peaks in a ~~FR~~ NMR Spectrum. They also contain a C=O ~~bond~~. double bond. Therefore for ~~a~~ ethylpropanoate this ~~would~~ will be represented by a peak in the range of 165-175ppm and in pentanoic acid would be in the range of 175-185ppm. Another characteristic which differentiates the two compounds is that ~~as~~ the ~~ester, ethylpropanoate, has a~~ carboxylic acid, pentanoic acid, has an -OH group whereas esters do not. Therefore this peak ~~represent~~ would be shown in the range of 50-65ppm. ~~Esters~~ The ~~R~~ Ethylpropanoate does not have

c) 

88 ethyl ethanoate



ethanoic acid.



ethanol

For Ethanoic acid is an carboxylic acid alcohol. ~~For the~~ It has 2 carbon environments which should equal the number of peaks present in the NMR spectrum. Ethanol is an alcohol is ~~has~~ with 2 carbon environments and for ethylethanoate there are 4 carbon environments. ~~Ethanol~~ Ethanoic acid and ethylethanoate both consist of C=O double bond where as ethanol it does not. Ethanol consists of an -OH group instead, therefore this peak would be shown ~~it~~ in the range of 50-65 ppm much like the ethanoic acid which also consists of an -OH group. However because Ethanol does not have a C=O double bond ~~bond~~ its NMR Spectrum would be G. This means that because ethanoic acid has two carbon environments and ethylethanoate has 4, this can be easily distinguished. For ethanoic acid the peak representing the C=O would be in the range 175 - 185 ppm.

This compound would be represented by H. This is because its C=O peak is represented at approximately 177 ppm. This leaves I to be ethylethanoate. I has 4 peaks, as the peak at approximately 77 ppm is not included as it is a solvent. These 4 peaks relates to the number of carbon environments. Its C=O is represented in the range of 165 - 175 ppm. In this case it ~~is~~ ~~the~~ is read approximately at 168 ppm.

For the IR Spectrum, ethylethanoate and ethanoic acid both have a C=O bond whereas ethanol does ~~and~~ not. ~~As~~ The C=O bond would be represented by a very narrow peak. For ethylethanoate this would be in the range of 1750 - ~~1735~~ 1735 cm^{-1} and ~~at~~ ethanoic acid it would be in ~~the~~ 1780 - 1710. But because the range of ethylethanoate is within the range of ethanoic acid, another characteristic is the -OH present in ethanoic acid and not in ethylethanoate.

	Grade Boundary: High Merit
2.	To meet Merit students need to demonstrate in-depth understanding of spectroscopic data in chemistry. The structures of organic molecules to spectroscopic data from different techniques have been linked. However, in Task (a) the structure of butanal is drawn rather than butanone. In Task (b) all three techniques have been linked in identifying which isomer is present. However, the justification for ethyl propanoate is incorrect. To meet Excellence the justification of the structure of organic molecules by integrating spectroscopic data from different techniques must be correct.

are 4 peaks meaning 4 carbon environments and therefore the NMR ~~a~~ agrees with C_4H_8O not C_5H_{12}.
This means that the compound could be:

(a)

$$CH_3CH_2CH_2\overset{O}{\overset{\|}{C}}-H$$

It is reasonable to assume that compound 2 could be butanone because butanone has 4 carbon environments which could be represented by the four peaks at about 210ppm, 35ppm, 30ppm, and 10ppm. Since butanone has a C=O double bond it agrees with the NMR spectrum which has a peak at 210 ppm this peak is the most downfield. The next most downfield is likely to be CH_2 as CH_2 is the next closest to the oxygen hence it would agree with the peak at about 35ppm, the next third most downfielded is likely to be then represented by another CH_2 as this is the 3rd furthest from the C=O. The last peak at about 10 ppm is then representative of the CH_3 group which is the least deshielded and the furthest from the C=O.

The IR spectrum also supports that the compound is a ketone and not a carboxylic acid as there is no characteristic O-H trough present. If OH bond was present then it would have produced a very broad O-H trough in the range 2500 - 3000 cm^{-1}, this is not there in the spectrum hence compound 2 cannot be a carboxylic acid or alcohol. There is a characteristic C-O carbon to oxygen double bond trough represented by the sharp trough at about 1700 cm^{-1}, this once again agrees with the fact that compound 2 is butanone as butanone has a C=O carbon to oxygen double bond.

b) $CH_3CH_2C(=O)OCH_2CH_3$ $CH_3CH_2CH_2CH_2C(=O)OH$

IR spectrum will show ~~a~~ the C=O carbon to oxygen double bond for both ethyl propanoate and pentanoic acid as both esters and carboxylic acids have a C=O bond. In the IR spectrum this for C=O carbon to oxygen double bond will produce a sharp trough in the range 1720 - 1735 cm-1 for an ester and in the range 1680 - 1710 cm-1 for a carboxylic acid. The position of this C=O carbon - oxygen bond varies depending on the sort of compound it is in. Even though C=O bond is present in both possible compounds, if the compound is ~~a~~ pentanoic acid the IR spectrum will also show a characteristic O-H ~~bon~~ trough. The O-H bond produces a easily recognisible, broad trough in the range 3000 - 3500 cm-1 this trough will not be produced ~~if~~ the compound is ethyl propanoate because esters do not have a O-H bond.

^{13}C NMR

In the NMR spectrum each peak identifies a carbon atom with a different environment within a molecule. If the compound is the ester ethyl propanoate which has 4 carbon environments, it will have 4 peaks whereas if the compound is the carboxylic acid pentanoic acid which has 5 carbon environments, it will have 5 peaks. ~~a~~ For both either compound the NMR spectrum will show a peak that is more downfield than the other peaks, this peak is due to the C=O carbon to oxygen double bond which is present in both ethyl propanoate and pentanoic acid, and will produce a peak that is more downfield in the range 165 - 175 cm-1 for ethyl propanoate and 175 - 185 cm-1 for pentanoic acid.

	Grade Boundary: Low Merit
3.	To meet Merit students need to demonstrate in-depth understanding of spectroscopic data in chemistry. In Tasks (a) and (c) the structure of the organic molecules has been linked to the spectroscopic data. However, there is no linking of the spectroscopic data from the different techniques to the structure of the organic molecules. To meet Merit more securely the structure of organic molecules must be linked to spectroscopic data from the different techniques.

Student 3: Low Merit

Task (a)

(i) It is determined from the peak most to the right on the spectrum

(ii) I think it is a compound with a carbonyl group as there is peak at 1600 cm^{-1}on the IR spectrum which is where the carbonyl peak is. It is not an alcohol as there is no broad OH group at 3000 cm^{-1}on the spectrum. There are 4 different carbon environments in the molecule, as shown by 4 peaks. It could be butanone or butanal as they both have 4 peaks, but probably butanone as a more downfield peak.

Task (b)

Mass spectrometry: the different molecules would produce different fragments and different base peaks as they would break at different places. They would both have the same molecular ion peak.

IR: Ethyl propanoate would have have a carbonyl group at 1700 cm^{-1} and an OH group broad at 3200 cm^{-1}. Pentanoic acid would only have the carbonyl group.

C-13 NMR: Both molecules would have 5 peaks but they would be in different places.

Task (c)

Mass spectra

A=ethyl ethanoate as the Molar mass and peak on right are the some

B=ethanoic acid

C=ethanol

IR

D=OH group only so it is ethanol

E=OH group and carbonyl group so it is ethanoic acid

F=no OH group so it is ethyl ethanoate

NMR

G=2 peaks so could be ethanol or ethanoic acid, must be ethanol as no really downfied peaks as ethanol does not have a carbonyl group

H=2 peaks so could be ethanol or ethanoic acid, one peak is more downfield so it must be the carbon with the carbonyl group in ethanoic acid

I=ethyl ethanoate

	Grade Boundary: High Achieved
4.	To meet Achievement students need to demonstrate understanding of spectroscopic data in chemistry. Discreet aspects of the structure have been correctly identified for the IR spectra only (Task c). The position of the OH group has been correctly identified for all three compounds using IR data. Correct terminology and units have been used. To meet Merit the structure of organic molecules to spectroscopic data from different techniques must be linked.

Student 4: High Achieved

Task C

IR

D= broad OH group at 3400cm^{-1} only so it is ethanol

E=OH group at 3400cm^{-1} and carbonyl group at 1750cm^{-1} so it is ethanoic acid

F=no broad OH group at 3400cm^{-1} and there is a sharp peak at 1750cm^{-1} which corresponds to a carbonyl group so it is ethyl ethanoate

	Grade Boundary: Low Achieved
5.	To meet Achievement students need to demonstrate understanding of spectroscopic data in chemistry. Discreet aspects of organic molecules have been identified. However, there is limited use of correct terminology and units (e.g. *D=OH group only so it is ethanol*). Also, the position of the OH group has not been indicated and what it would look like. The number of different carbon environments in a molecule is identified and related to the number of peaks in C13 NMR. To meet Achievement more securely there must be correct use of terminology and units. The position of the OH group must also be indicated (i.e. peaks in IR spectra and links to bonds or functional groups).

Student 5: Low Achieved

Task (a)

(iii) It is determined from the peak most to the right on the spectrum

(iv) I think it is a compound with a carbonyl group as there is peak at 1600 on the IR spectrum which is where the carbonyl peak is. It is not an alcohol as there is no OH group on the spectrum. There are 4 different carbon environments in the molecule.

Task (b)

Mass spectrometry: the different molecules would produce different fragments and different base peaks as they would break at different places. They would both have the same molecular ion peak.

IR: Ethyl propanoate would have have a carbonyl group at 1700 and an OH group broad at 3200. Pentanoic acid would only have the carbonyl group.

C-13 NMR: Both molecules would have 5 peaks but they would be in different places.

Task (c)

Mass spectra

A=ethyl ethanoate as the Molar mass and peak on right are the some

B=ethanoic acid

C=ethanol

IR

D=OH group only so it is ethanol

E=OH group and carbonyl group so it is ethanoic acid

F=no OH group so it is ethyl ethanoate

NMR

G=2 peaks so could be ethanol or ethanoic acid

H=2 peaks so could be ethanol or ethanoic acid

I=ethyl ethanoate

	Grade Boundary: High Not Achieved
6.	To meet Achievement students need to demonstrate understanding of spectroscopic data in chemistry. There are some partial correct points but not substantial enough, e.g. where would the peaks be on an IR spectrum. Some information is incorrect, e.g. Task a (ii). There is an attempt at identifying discreet aspects of the structure of organic molecules. To meet Achievement there should be correct identification of discrete aspects of the structure of organic molecules using one piece of spectroscopic data.

Student 6: High Not Achieved

Task (a)

(i) The mass is 72

(ii) It is not an alcohol from the IR spectrum and there are 5 different peaks so there are 5 different carbons but we must take away the solvent peak so there are 4.

Task (b)

Mass spectrometry: They would both have the same molar mass but break in different places.

IR: Ethyl propanoate would have have a carbonyl group and an OH group broad at 3200. Pentanoic acid would only have the carbonyl group.

C-13 NMR: They would have different peaks as there are different carbon envirmonments.

C-13 NMR: Both molecules would have 5 peaks but they would be in different places.

Task (c)

Mass spectra

A=ethyl ethanoate as the Molar mass and peak on right are the some

B=ethanoic acid

C=ethanol

IR

D=OH group only so it is ethanol

E=OH group and carbonyl group so it is ethanoic acid

F=no OH group so it is ethyl ethanoate

NMR

G=2 peaks so could be ethanol or ethanoic acid, must be ethanol as no really downfied peaks as ethanol does not have a carbonyl group

H=2 peaks so could be ethanol or ethanoic acid, one peak is more downfield so it must be the carbon with the carbonyl group in ethanoic acid

I=ethyl ethanoate