

NZQA Approved

Internal Assessment Resource

Chemistry Level 3

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| This resource supports assessment against:  Achievement Standard 91388  Demonstrate understanding of spectroscopic data in chemistry |
| Resource title: Identifying the reaction products |
| 3 credits |
| This resource:   * Clarifies the requirements of the Standard * Supports good assessment practice * Should be subjected to the school’s usual assessment quality assurance process * Should be modified to make the context relevant to students in their school environment and ensure that submitted evidence is authentic |

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| Date version published by Ministry of Education | February 2017 Version 2  To support internal assessment from 2017 |
| Quality assurance status | These materials have been quality assured by NZQA. NZQA Approved number A-A-02-2017-91388-02-6372 |
| Authenticity of evidence | Teachers must manage authenticity for any assessment from a public source, because students may have access to the assessment schedule or student exemplar material.  Using this assessment resource without modification may mean that students’ work is not authentic. The teacher may need to change figures, measurements or data sources or set a different context or topic to be investigated or a different text to read or perform. |

Internal Assessment Resource

Achievement Standard Chemistry 91388: Demonstrate understanding of spectroscopic data in chemistry

Resource reference: Chemistry 3.2B v2

Resource title: Identifying the reaction products

Credits: 3

Teacher guidelines

The following guidelines are supplied to enable teachers to carry out valid and consistent assessment using this internal assessment resource.

Teachers need to be very familiar with the outcome being assessed by Achievement Standard Chemistry 91388. The achievement criteria and the explanatory notes contain information, definitions, and requirements that are crucial when interpreting the Standard and assessing students against it.

Context/setting

This activity requires students to interpret spectral data to determine the identity of discrete aspects of the structure of an organic compound. The data will be provided for the students. They will interpret each piece of data and combine the information to determine the structure of the organic molecule. Information about the empirical formula of the molecule will be provided.

Conditions

It is suggested that this assessment task will take place over 1-2 class periods. Students will be able to use annotated data tables for IR absorption frequencies and 13C NMR chemical shifts.

Resource requirements

Tables for IR absorption frequencies and 13C NMR chemical shifts.

Data sheet: Synthesis of ethyl ethanoate.

Additional information

Before students can realistically attempt to use spectral data, they need to be familiar with the structures of organic molecules, including functional groups and isomers, as required by Achievement Standard 3.5. However, it would be possible to work with Level 2 compounds but this restricts the range of possible compounds that can be used in the assessment tasks.

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Achievement Standard Chemistry 91388: Demonstrate understanding of spectroscopic data in chemistry

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Resource title: Identifying the reaction products

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| Achievement | Achievement with Merit | Achievement with Excellence |
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| Demonstrate understanding of spectroscopic data in chemistry. | Demonstrate in-depth understanding of spectroscopic data in chemistry. | Demonstrate comprehensive understanding of spectroscopic data in chemistry. |

Student instructions

Introduction

This assessment activity requires you to determine the structure of organic compounds, using mass spectra, IR sprecta, and 13C NMR spectra and to justify how the spectroscopic data were used to determine the structure.

This is an individual task and will take place over 1-2 class periods.

You will be assessed on the comprehensiveness of your understanding of spectroscopic data in chemistry.

Task

Part 1

While working on an organic synthesis, a research chemist isolated a compound (Z). Mass spectrometry revealed that compound Z had *M*r of 72. From this analysis, the student proposed that the structure could be either C5H12or C4H8O. Compound Z does not have a ring in its structure.

a) Explain how mass spec data gives the *M*r of the compound.

b) The IR and 13C NMR spectra were obtained from Z. Deduce a possible structure for Z indicating clearly the evidence that you have used from each spectrum.



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(Note that the peak at 75 ppm is a solvent peak.)

Part 2

You have been asked to analyse the product of a chemical synthesis. The empirical formula for the product is C5H10O2. You suspect that the product is ethyl propanoate or pentanoic acid.

Outline how data collected using mass spectrometry, infra-red spectrometry, and 13C NMR can be used to determine which of the two isomers is present.

You should compare and contrast the spectra for each isomer from each of the three techniques and explain how combining all the evidence will allow you to decide which isomer is present.

Part 3

An attempted synthesis of ethyl ethanoate was carried out by heating ethanoic acid and ethanol under reflux in the presence of concentrated sulfuric acid. The organic product is distilled and analysed by spectroscopy to ascertain if the reaction has taken place.

The equation for the reaction is:

Mass spectrometry, infra-red spectrometry, and 13C NMR data are provided for each of the reactants and the organic product of this reaction.

For each type of spectra provided (A – I), identify the compound from which the spectrum would have been obtained. Justify your answer by comparing and contrasting each set of spectra, discussing the significant peaks and linking these to the molecular structure of each compound.

Assessment schedule: Chemistry 91388 Identifying the reaction products

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| Evidence/Judgements for Achievement | Evidence/Judgements for Achievement with Merit | Evidence/Judgements for Achievement with Excellence |
| The student identifies discrete aspects of the structure of organic compounds using spectroscopic data. For a given structure, the student identifies discrete aspects for all three spectra:   * the molecular ion in mass spec data * key peaks in IR spectra and links to functional groups * the number of different carbon environments in a molecule and relates these to 13C NMR.   Evidence could be found from annotated spectra. | The student interprets spectra and determines the structure of an organic compound.  The student links the key aspects of all three spectra to the structure.  For example:   * for Part 1, the student gives one of the two possible formulae for the compound and links this to the peaks present in the IR and 13C NMR spectra (discussion about other possible functional groups is missing) * for Parts 2 and 3, the student recognises most of the key features of the spectra but does not integrate all the spectra to show how the two compounds could be distinguished.   *The examples above relate to only part of what is required, and are just indicative.* | The student has interpreted spectra to solve the structure of a molecule.  The student justifies the structure of an organic molecule by integrating spectroscopic data.  **Part 1**  ***Z* is**  It is not possible to distinguish between these on the basis of the spectra given.  *Mass spec* – will have a molecular ion, M+, at 72 since both compounds have *Mr* = 72.  *IR* – peak at 1750 cm-1 evidence of C=O bonding (C4H8O not C5H12).  No diffuse peak at around 3200 cm-1 so no O-H stretching. No peak in 1250 cm-1 so no evidence of C-O. (No evidence of C=C as C-H peak is below 3000 cm-1).  *13C NMR* – 4 peaks with one peak downfield (220 ppm) providing further evidence of a carbonyl (C=O).  IR and NMR give evidence for C=O so compound has formula C4H8O rather than C5H12. (Other compounds with this formula ruled out on the basis of no evidence for C=C double bond or -OH). Structure could be **butanone** **or butanal** both of which C=O and 4 different C environments with the C=O peak being downfield from the other 3.  **Part 2**  *Mass spec* – same molecular ion peak for both compounds expected at 102. (*M*(C5H10O) = 102 g mol-1).  However, there will be variation in the fragment peaks. For example for the ester there would a significant peak expected at *M* = 57 for the fragment CH3CH2C=O which would not be present in the acid spectrum.  *IR* – acid will have a broad peak at 3500 cm-1 for -OH stretching and a strong peak at 1725 cm-1 C=O  – ester will have strong peak around 1750 cm-1 for C=O and at around 1200 cm-1 for C-O.  *13C NMR* – 5 peaks for both compounds with the C=O for the acid occurring further downfield than for the ester for the acid. For both compounds, there are 5 different carbon environments hence 5 different peaks.  Evidence for the functional group comes from the IR and this will be supported by the position of the downfield shift for the C=O carbon in the 13C NMR and the fragment pattern in the mass spec.  **Part 3**  *Mass spectra*  A = ethyl ethanoate – M+ at 90, peak at 43 for CH3C=O fragment  B = ethanoic acid – M+ at 60, peak at 43 for CH3C=O fragment  C = ethanol – M+ at 46, peak at 31 for CH2OH fragment.  *IR spectra*  D = ethanol – diffuse peak at 3400 cm-1 suggests O-H stretching  E = ethanoic acid – broad peak at 3100 cm-1 is -OH and at 1700cm-1 is C=O so suggests carboxylic acid  F = ethyl ethanoate – peak at 1750 cm-1 for C=O and at 1250 cm-1 for C-O  All IR spectra have similar fingerprint areas – peak at 3000 cm-1 is from C-H bonding.  *13C NMR spectra*  G = ethanol – 2 carbon atom environments so 2 peaks  H = ethanoic acid 2 carbon atom environments so 2 peaks, one shifted downfield for C=O  I = ethyl ethanoate – 4 carbon atom environments so 4 peaks, one shifted downfield for C=O.  Discussion links the three different types of spectra for each compound to the structural formula.  *The examples above relate to only part of what is required, and are just indicative.* |

Final grades will be decided using professional judgement based on a holistic examination of the evidence provided against the criteria in the Achievement Standard.