WJEC (Wales) Chemistry A-level

Topic 2.8 - Instrumental Analysis

Flashcards

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What analytical processes can be used to identify compounds and calculate their molecular formula?

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What analytical processes can be used to identify compounds and calculate their molecular formula?

- Mass spectroscopy
- Infrared spectroscopy
- Proton NMR spectroscopy
- C^{13} NMR spectroscopy

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Briefly describe what happens during mass spectrometry

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Briefly describe what happens during mass spectrometry

A vaporised sample of atoms of molecules is ionised into positive ions. The ions are accelerated, deflected by a magnetic field and then detected. This produces a graph with mass to charge ratio (m/z) on the x axis and relative abundance on the y axis.

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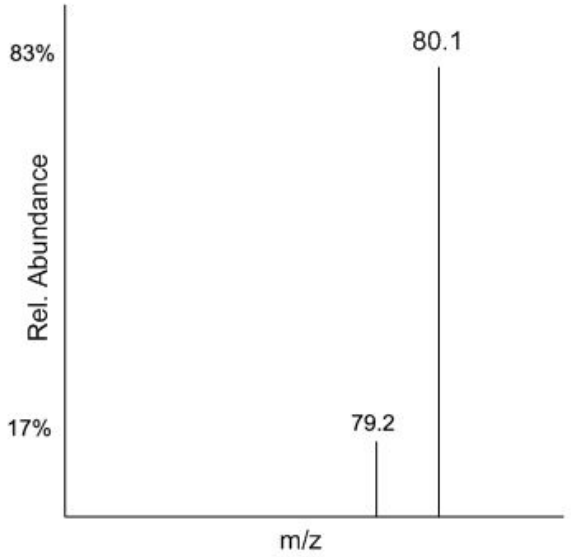
Use the graph to calculate the relative atomic mass of this substance



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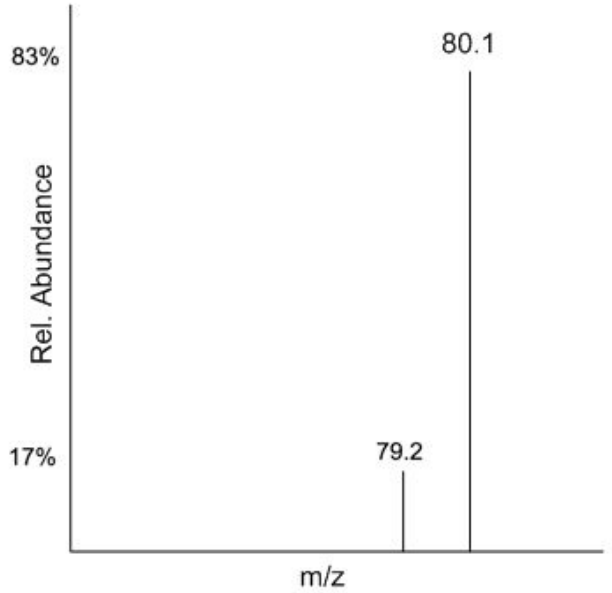
Use the graph to calculate the relative atomic mass of this substance

$[(79.2 \times 17) + (80.1 \times 83)] \div 100$

$= 79.95 \text{ g mol}^{-1}$



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How can you use a mass spectrum to deduce the relative molecular mass of a sample of a compound?

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How can you use a mass spectrum to deduce the relative molecular mass of a sample of a compound?

The peak with the highest m/z value (the molecular ion peak, M^+) is caused by the whole molecule, therefore that m/z value = molecular mass.

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‘Ions in a mass spectrometer can have a 2+ charge’
True or False?

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‘Ions in a mass spectrometer can have a 2+ charge’ True or False?

TRUE

Ions in a mass spectrometer can have a 2+ charge, but the 1+ charge is more common.

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Chlorine has two possible isotopes, Cl^{35} with a 75% abundance and Cl^{37} with a 25% abundance. Predict what the mass spectrum would look like for the diatomic molecule.

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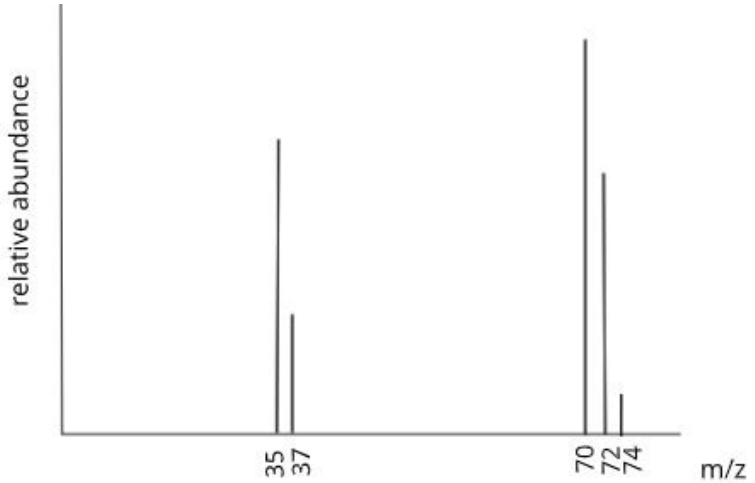
Chlorine has two possible isotopes, Cl^{35} with a 75% abundance and Cl^{37} with a 25% abundance. Predict what the mass spectrum would look like for the diatomic molecule.

Possible combinations of the Cl_2^+ :

- 35+35=70
- 35+37=72
- 37+37=74



The 70:72:74 is in the ratio 9:6:1.

Some fragmentation occurs so there are also peaks at m/z 35 and 37.

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What happens when infrared radiation is directed at a compound?

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What happens when infrared radiation is directed at a compound?

Bonds within the molecule absorb specific frequencies of radiation.

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What happens when specific frequencies of radiation are absorbed by bonds in a molecule?

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What happens when specific frequencies of radiation are absorbed by bonds in a molecule?

The bonds vibrate. This causes the bond to stretch or bend.

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What can be identified using peaks on an infrared spectrum? How?

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What can be identified using peaks on an infrared spectrum? How?

The functional groups within a molecule can be identified by comparing the peaks to known values in a data book.

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What is the fingerprint region on an infrared spectrum?

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What is the fingerprint region on an infrared spectrum?

The region typically between 1500 cm^{-1} and 500 cm^{-1} that contains a complicated pattern of absorptions. Every compound has a unique fingerprint region.

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Why can ^{13}C nuclei be used in NMR spectroscopy?

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Why can ^{13}C nuclei be used in NMR spectroscopy?

^{13}C nuclei can align with or against a magnetic field. The nuclei are less stable when opposing the magnetic field meaning this alignment has higher energy. Energy can be supplied to the nucleus in the form of radio waves and cause it to flip from the more stable alignment to the less stable alignment. This energy change depends on the carbon environment.

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What is a carbon environment?

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What is a carbon environment?

The atoms, or groups of atoms, that a carbon atom is bonded to.

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What can be deduced from a carbon-13 NMR spectrum? How?

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What can be deduced from a carbon-13 NMR spectrum? How?

Number of different carbon environments = number of peaks on the spectrum.

Types of carbon environments - compare the chemical shift values of the peaks to the data book to identify the carbon environments.

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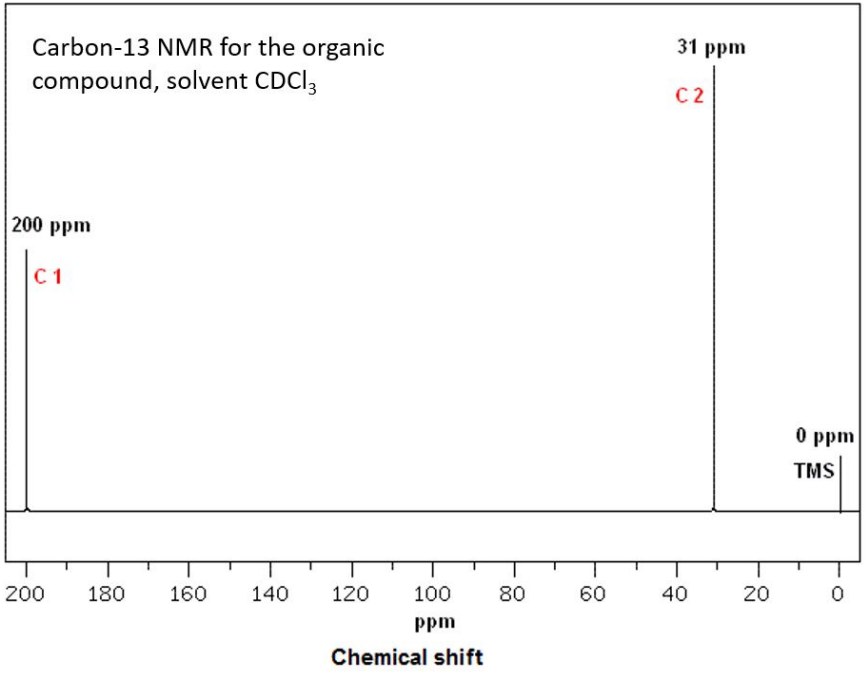
An organic compound contains two carbons and has the ^{13}C NMR spectrum shown. Determine its structure.



'File:13C NMR ethanal.GIF', Wikimedia Commons

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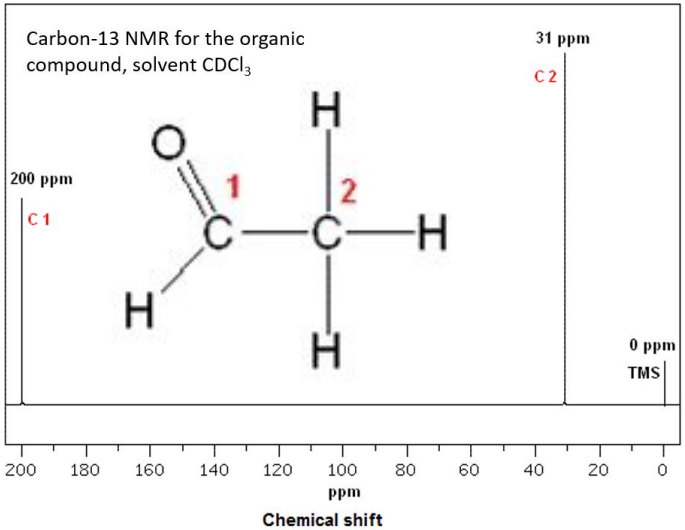
An organic compound contains two carbons and has the ^{13}C NMR spectrum shown. Determine its structure.

- The compound has 2 carbons.
- There is a peak at 200 ppm meaning the compound must contain C=O.
- The spectrum shows 2 peaks so there are 2 different carbon environments. Both carbons are in different environments.
- The chemical is ethanal.

'File:13C NMR ethanal.GIF', Wikimedia Commons CC0 1.0



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Predict the number of peaks in the ^{13}C NMR spectrum for 3-methylbutanal

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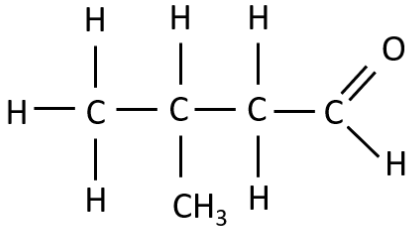
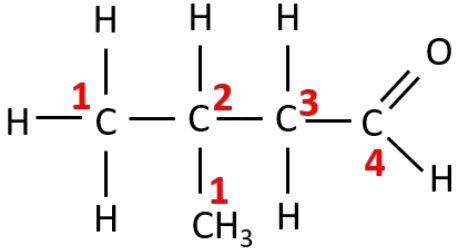
Predict the number of peaks in the ^{13}C NMR spectrum for 3-methylbutanal

Structure:



Number the carbon environments:



There are 4 environments so there will be 4 peaks.

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Why can protons be used in NMR spectroscopy?

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Why can protons be used in NMR spectroscopy?

Hydrogen nuclei can align with or against a magnetic field. The direction of this alignment can be flipped using a specific frequency of radio waves (known as resonance condition). This is because there is a difference in the energy of the two alignments. The frequency required for this change depends on the proton environment.

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How can a proton environment be identified using a proton NMR spectrum?

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How can a proton environment be identified using a proton NMR spectrum?

Compare the chemical shift values of the peaks to values in the data book.

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On a proton NMR spectrum, what does the ratio of the areas under the peaks indicate?

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On a proton NMR spectrum, what does the ratio of the areas under the peaks indicate?

The relative number of protons in each environment.

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What are equivalent protons?

CC BY NC ND

What are equivalent protons?

Protons in the same environment. These may be on the same or different carbons.

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What does the splitting pattern of peaks on a proton NMR spectrum show?

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What does the splitting pattern of peaks on a proton NMR spectrum show?

The number of protons on the adjacent carbon atoms.

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Name the first 4 splitting patterns on a proton NMR spectrum

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Name the first 4 splitting patterns on a proton NMR spectrum

Singlet (1 peak)

Doublet (2 peaks)

Triplet (3 peaks)

Quartet (4 peaks)

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What is the n+1 rule?

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What is the n+1 rule?

The number of peaks in the splitting pattern is equal to the number of adjacent protons (n) plus one.

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When doesn't the n+1 rule work?

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When doesn't the n+1 rule work?

- Alcohols - the chemical shift for the hydrogen atom in -OH is variable and this peak is always a singlet. -OH doesn't cause splitting in adjacent hydrogens.
- Equivalent hydrogens - protons bonded to the same carbon (protons in the same environment) have no effect on each other in terms of splitting.
- Benzene - the splitting pattern is very complicated (called a multiplet). The peaks for a benzene ring will be found in the range 6.0-9.0 ppm.

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What does the peak at 0 ppm on a proton NMR represent?

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What does the peak at 0 ppm on a proton NMR represent?

TMS (tetramethylsilane)

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What is TMS used as?

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What is TMS used as?

The standard for chemical shift measurements during NMR spectroscopy.

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Why is TMS used as the standard for chemical shift measurements in NMR spectroscopy?

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Why is TMS used as the standard for chemical shift measurements in NMR spectroscopy?

- It has 12 hydrogens in the same environment meaning a single strong peak will be produced in proton NMR.
- It contains carbon and hydrogen atoms meaning it can be used in both carbon and proton NMR.
- It contains 1 carbon environment meaning it produced a single peak in ^{13}C NMR.
- It's non-toxic.
- It's inert so won't react with the compounds under analysis.

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