CAIE Chemistry A-level

Topic 22 - Analytical Techniques

Flashcards

What happens when infrared radiation is directed at a compound?

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Bonds within the molecule absorb specific frequencies of radiation.

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

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

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

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

What is the fingerprint region on an infrared spectrum?

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

Briefly describe what happens during mass spectrometry

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A vaporised sample of atoms of molecules is turned 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.

What is the molecular ion (M^+) peak on a mass spectrum?

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The peak with the greatest mass to charge ratio. The molecular mass of a compound is equal to the m/z value of this peak.

What is the M^{+1} peak on a mass spectrum? What is it caused by?

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A tiny peak 1 unit to the right of the molecular ion peak. This is caused by the presence of the ^{13}C isotope (relative abundance 1.11%). ^{13}C has one more neutron than ^{12}C meaning that the relative formula mass is increased by 1.

How can the relative heights of the M^{+} and M^{+1} peaks be used to predict the number of carbon atoms in a molecule?

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n is the number of carbon atoms

$$n = \frac{100}{1.1} \times \frac{\text{abundance of } M^{+1} \text{ ion}}{\text{abundance of } M^{+} \text{ ion}}$$

When would an M^{+2} peak be seen on a mass spectrum?

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When a compound contains a chlorine or bromine atom.

Describe how the presence of a chlorine atom in a compound causes a M^{+2} peak on the mass spectrum

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In these compounds, chlorine exists as two isotopes: ^{35}Cl or ^{37}Cl. Compounds containing the ^{37}Cl isotope will have a relative formula mass that is 2 units larger than compounds containing the ^{35}Cl isotope, causing the M^{2+} peak.

What is the ratio of the peak heights of the M^{+} and M^{+2} peaks on the mass spectrum of a compound containing chlorine? Why?

What is the ratio of the peak heights of the M^{+} and M^{+2} peaks on the mass spectrum of a compound containing chlorine? Why?

3:1

Chlorine is 3 times more likely to be ^{35}Cl than ^{37}Cl.

Describe how the presence of a bromine atom in a compound causes an M^{+2} peak on the mass spectrum

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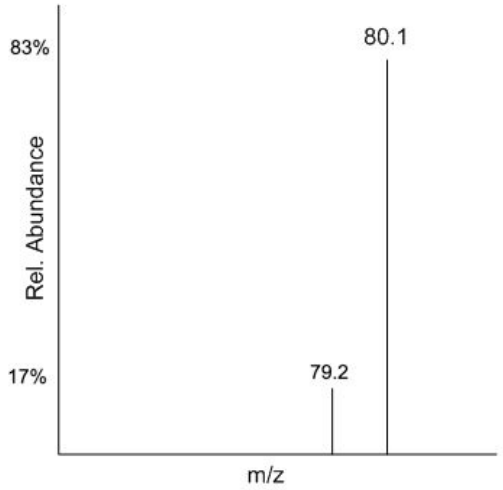
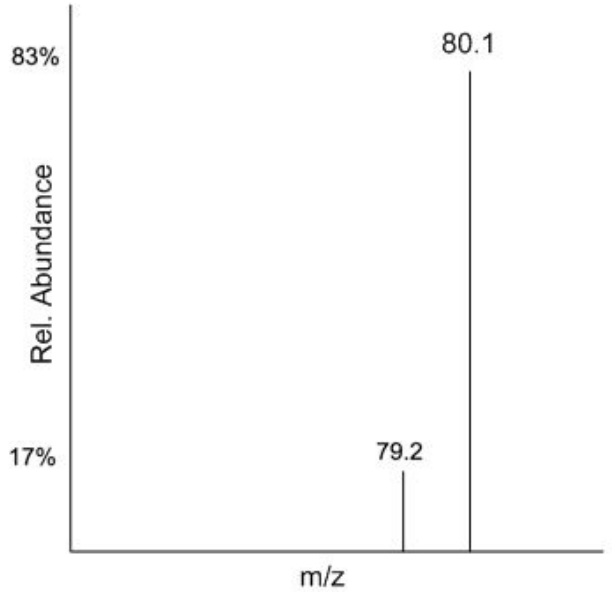
Bromine exists as two isotopes: ^{79}Br or ^{81}Br. Compounds containing the ^{81}Br isotope will have a relative formula mass that is 2 units larger than compounds containing the ^{79}Br isotope, causing the M^{2+} peak.

Using the mass spectrum below, what is the relative abundance of the isotope with a relative isotopic mass of 80.1?

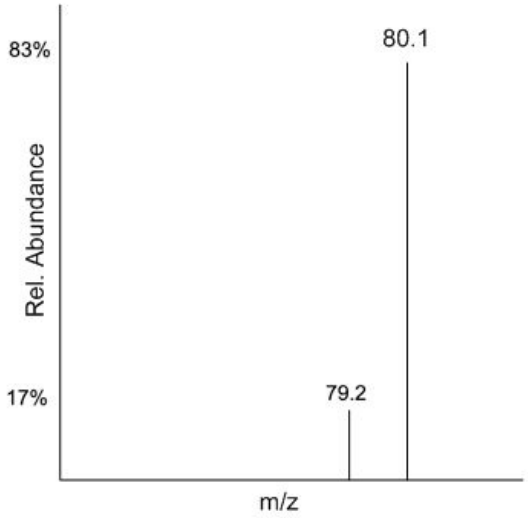


Using the mass spectrum below, what is the relative abundance of the isotope with a relative isotopic mass of 80.1?

83%



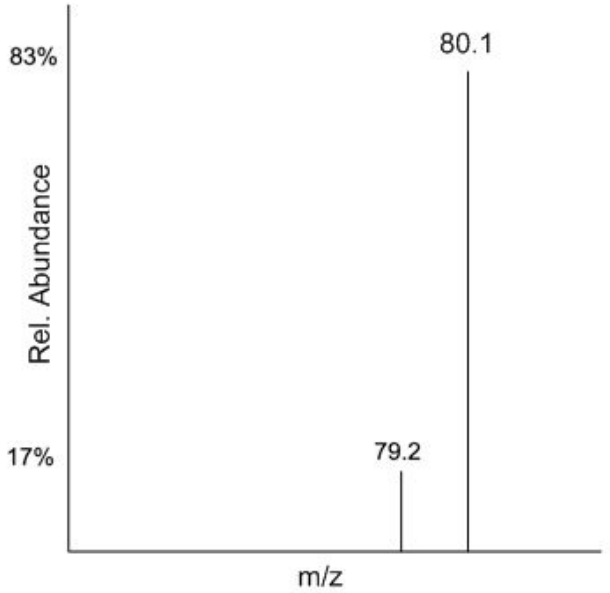
Use the mass spectrum below to deduce the relative atomic mass of the sample



Use the mass spectrum below to deduce the relative atomic mass of the sample

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

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



How can a mass spectrum be used to deduce the relative molecular mass?

How can a mass spectrum be used to deduce the relative molecular mass?

The peak with the highest m/z value (the molecular ion peak or M^+ peak) is caused by the whole molecule after one electron has been knocked off.

m/z value of M^+ peak = molecular mass

How many molecular peaks will a compound containing three chlorine atoms have?

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Four molecular peaks. There are two isotopes of chlorine so there a four different combinations:

35 + 35 + 35

35 + 35 + 37

35 + 37 + 37

37 + 37 + 37

Describe the formation of fragment ions during mass spectrometry

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Fragment ions form when an unstable molecular ions break down into a positive ion and an uncharged free radical.

$$M^+ \rightarrow X^+ + Y\bullet$$

What is a free radical?

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A species with an unpaired electron.

Why are the free radicals formed during the fragmentation of molecular ions not shown as peaks on the mass spectrum?

Why are the free radicals formed during the fragmentation of molecular ions not shown as peaks on the mass spectrum?

These free radicals are uncharged. Only charged particles are detected.

How can a fragment ion be identified from a mass spectrum?

How can a fragment ion be identified from a mass spectrum?

Compare the m/z value of the fragment ion peak with the relative formula masses of possible fragment ions.