OCR (B) Chemistry A-Level
PL8 - Modern Analytical Techniques
Flashcards

How do you calculate the molecular formula from the M⁺ peak on a mass spectrum?

How do you calculate the molecular formula from the M+ peak on a mass spectrum?

- The M^+ peak will tell you the M_r of the compound.
- Find the number of empirical formula units per molecule:
- M_r ÷ empirical mass.
- Multiply this number by the empirical formula to get the molecular formula.

What is the difference in mass between peaks due to?

What is the difference in mass between peaks due to?

- The loss of groups of atoms.
- These fragments can be analysed to help deduce the structure of the molecule.

What is carbon-13 NMR?

What is carbon-13 NMR?

- A C^{13} spectrum will tell you the number of carbon environments (number of peaks = number of carbon environments).

- It will also tell you the types of each carbon environment present. Each carbon environment will have a chemical shift value. Compare this to chemical shift values found in your data sheet to identify the type of environment.
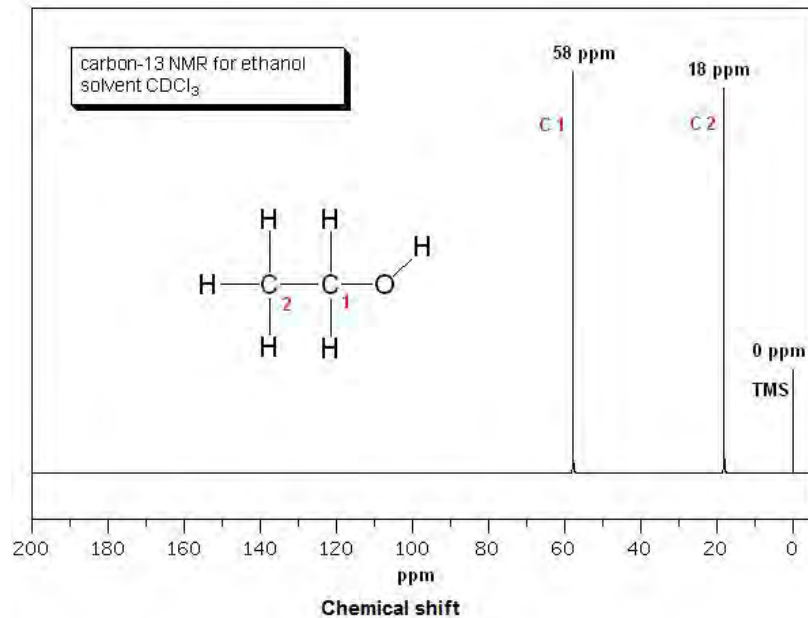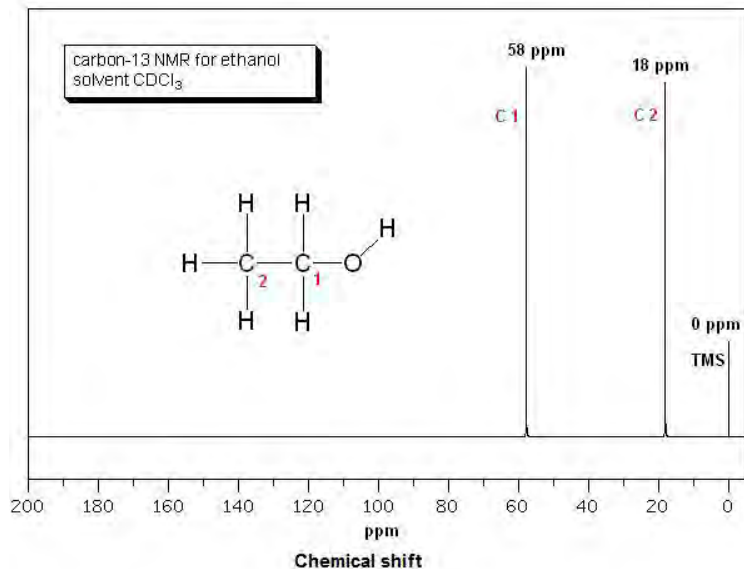
How do you identify the types of carbon environments present from a C^{13} spectrum?

How do you identify the types of carbon environments present from a C13 spectrum?

Carbon environment	Chemical shift /ppm	Type of environment
C1	58	C-O
C2	18	C-C

carbon-13 NMR for ethanol solvent $CDCl_3$

What is proton NMR?

What is proton NMR?

A proton NMR spectrum provides 4 important bits of information:

- The number of different proton environments.
- The types of proton environments present.
- The relative number of protons present in each environment.
- The number of protons present in different environments adjacent to a given proton environment.

How can you use a proton NMR spectrum to determine the number of different proton environments in a molecule?

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The number of peaks in the spectrum = the number of different proton environments.

How can you use a proton NMR spectrum to determine the types of proton environments present in a molecule?

How can you use a proton NMR spectrum to determine the types of proton environments present in a molecule?

Look at the chemical shift values and find the corresponding groups/proton environments on your data sheet.

How can you use a proton NMR spectrum to determine the relative number of protons present in each environment?

How can you use a proton NMR spectrum to determine the relative number of protons present in each environment?

This is normally done using an integration trace and so the relative peak areas will be provided and are usually written on the spectrum.

What can you determine from the splitting pattern of a proton NMR spectrum?

What can you determine from the splitting pattern of a proton NMR spectrum?

- Using the '$n+1$' rule you can determine the number of protons present in a different environment adjacent to a given proton environment.
- For a proton with n protons bonded to an adjacent carbon atom, the peak will be split into n+1.
- I.e. for a quartet splitting pattern, this proton environment will likely be adjacent to a $-CH_3$ group.

How do you use a combination of spectroscopic techniques to determine the structure of organic molecules?

How do you use a combination of spectroscopic techniques to determine the structure of organic molecules?

1. Mass spectrum (to determine molecular formula).

2. Infrared spectrum (to determine type of molecule/functional group).

3. C^{13} NMR spectrum & H^+ NMR spectrum (to determine the exact structure of the molecule).