Chemguide - questions

FRAGMENTATION PATTERNS

1. The mass spectrum of pentane looks like this:

simplified mass spectrum of pentane - CH3CH2CH2CH2CH3



- a) What causes the peak at m/z = 72?
- b) What causes the peak at m/z = 57?
- c) Write an equation to show how the species (molecule or ion) you quoted in part (b) is formed.
- d) What causes the peak at m/z = 43?
- e) Write an equation to show how the species you quoted in part (d) is formed.
- f) What causes the peak at m/z = 29?
- g) Write an equation to show how the species you quoted in part (f) is formed.
- 2. The mass spectrum of 2-methylbutane, an isomer of pentane, looks like this:



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The peak at m/z = 57 is much taller in 2-methylbutane than in its isomer pentane. Explain as fully as you can why this is, including an equation for the fragmentation that leads to it.

3. The mass spectra below are for pentan-2-one and pentan-3-one, but not necessarily in that order.

Pentan-2-one is CH₃COCH₂CH₂CH₃. Pentan-3-one is CH₃CH₂COCH₂CH₃.



Without looking back at the Chemguide page, decide which is which, explaining your thinking as fully as possible.