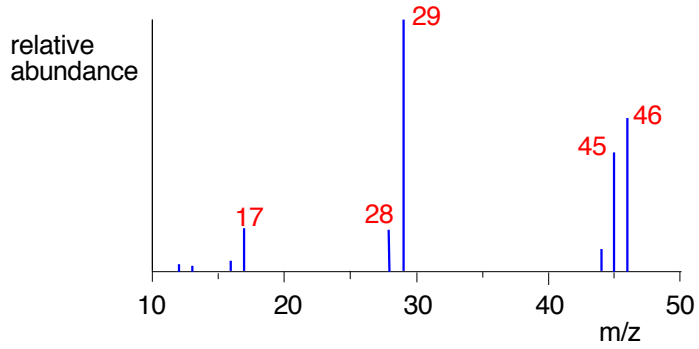
MASS SPECTRA: THE M+ LINE

1. The mass spectrum of a mystery compound below is a simplified version from the NIST WebBook. The figures in red show the m/z values for a few of the lines.



a) What is the m/z value for the molecular ion?

b) There are several organic compounds which have a molecular ion with that value. Use the approximate values for the relative isotopic masses in the table below to find as many of these compounds as you can.

You should draw the full structural formulae of each compound so that you are sure that such a compound can exist. For example, you might think that C_3H_{10} would be a possible compound, but any attempt to draw a structure would show that to be impossible.

c) A high resolution mass spectrum for this compound has an M+ line at m/z = 46.0054. Which of the structures that you have drawn in part (b) corresponds to this compound? (Note: If you don't have a compound which gives this value, then you have missed at least one! Think again.)

d) Write an equation to show the formation of the molecular ion from this compound.

e) Only attempt this question if you already know about fragmentation patterns. If you don't, come back to it later.

What fragments are represented by the lines at 17, 28, 29 and 45?

	approximate relative isotopic mass	accurate relative isotopic mass
^{1}H	1	1.0078
^{12}C	12	12.0000
^{14}N	14	14.0031
^{16}O	16	15.9949
^{19}F	19	18.9984