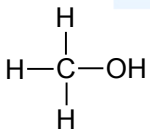
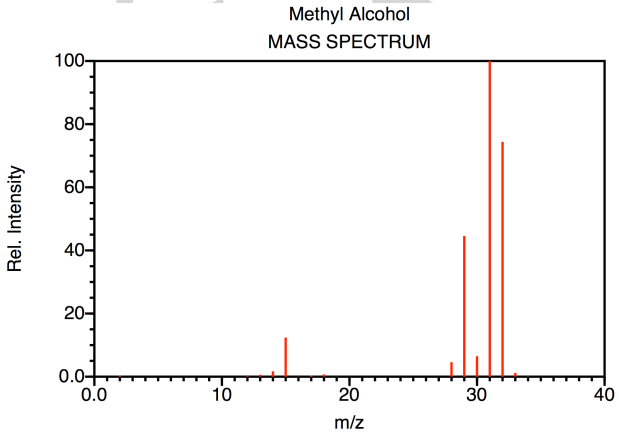
ORGANIC WORKSHEET 05e: Mass Spectrometry

As in the analysis of a single element's isotopes, the difference in mass between different fragments of more complicated molecules can be analyzed by mass spectrometry. This technique is widely used in the analysis of organic compounds (compounds of carbon), and the process follows a similar pattern to that used for isotopic analysis. The sample under analysis is ionized by knocking off an electron, thus creating what is known as the molecular ion, M^+. The molecular ion will be the heaviest of the fragments seen in the mass spectrum and will have a mass equivalent to the molecular mass of the sample. From there, at least two other things may be observed.

- The molecular ion will split up into various fragments, with each fragment having a mass smaller than M^+ that will create a line in the mass spectrum at M-X where X is an number that represents the mass of the atoms 'lost' from the fragment
- If the compound contains an element like Cl or Br that has two isotopes, a peak at M^+ and *another* peak at M+X may be observed. For Cl and Br, since Cl's isotopes are 35 and 37 and Br's are 79 and 81, the extra peak is observed at M+2

1. Consider the compound methanol (CH_3OH) shown below, and its mass spectrum.





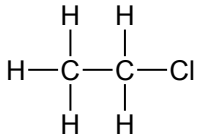
http://webbook.nist.gov/cgi/cbook.cgi?Spec=C67561&Index=0&Type=Mass&Large=on&SVG=on

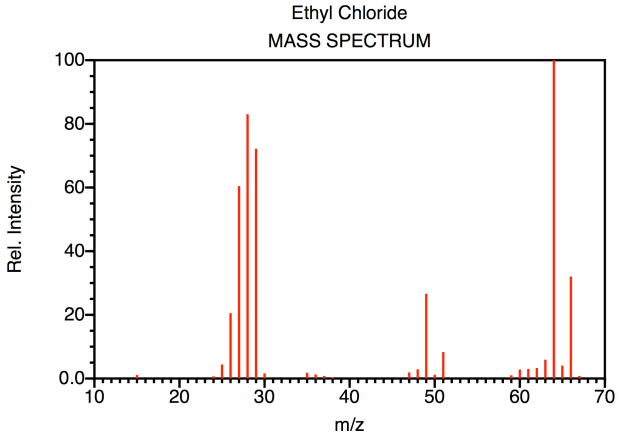
(a) Identify the M^+, molecular ion peak. (1)

(b) Suggest the fragment that is causing the peak at M-1. (1)

(c) Suggest the fragment that is causing the peak at m/z = 15. (1)

2. Consider the compound chloroethane (C_2H_5Cl) shown below, and its mass spectrum.





http://webbook.nist.gov/cgi/cbook.cgi?Spec=C75003&Index=0&Type=Mass&Large=on&SVG=on

(a) Identify the species that create the peaks at m/z 64 and m/z 66 respectively. Explain the existence of two peaks in this region of the spectrum. (3)

(b) Identify the peak at m/z = 29. (1)

(c) Identify the peak at m/z = 28. (1)