Figure 1 and the isotope abundance data from Table 1, we can see that there are 1.08 $^{13}\text{C}$ atoms for every 100 $^{12}\text{C}$ atoms, and the $^{13}\text{C}$ peak will be 1.08% as large as the $^{12}\text{C}$ peak.

The example above is simple, but the same methods can be applied to determine isotope peaks in more complicated molecules as well. The molecule C$_4$Br$_1$O$_2$H$_5$ has several isotope effects: $^{13}\text{C}$, $^2\text{H}$, $^{81}\text{Br}$, $^{17}\text{O}$, and $^{18}\text{O}$ all must be taken into account. First we will look at the (M+1)$^+$ peak in comparison with the M$^+$ peak. Only isotopes that will increase the value of M by 1 must be taken into consideration here – since $^{81}\text{Br}$ and $^{18}\text{O}$ would both increase M by 2, they can be ignored (the most abundant isotopes for Br and O are $^{79}\text{Br}$ and $^{16}\text{O}$). Like the previous example, there are 1.08 $^{13}\text{C}$ atoms for every 100 $^{12}\text{C}$ atoms. However, there are 4 carbon atoms in our molecule, and any one of them being a $^{13}\text{C}$ atom would result in a molecule with mass (M+1). So it is necessary to multiply the probability of an atom being a $^{13}\text{C}$ atom by the number of C atoms in the molecule. Therefore, we have:

\[
4\text{C} \times 1.08 = 4.32 = \text{molecules with a }^{13}\text{C atom per 100 molecules}
\]

We can repeat this analysis for $^2\text{H}$ and $^{17}\text{O}$:

\[
5\text{H} \times 0.015 = 0.075 = \text{molecules with a }^2\text{H atom per 100 molecules}
\]

\[
2\text{O} \times 0.04 = 0.08 = \text{molecules with a }^{17}\text{O atom per 100 molecules}
\]

Any of the three isotopes, $^{13}\text{C}$, $^2\text{H}$, or $^{17}\text{O}$ occurring in our molecule would result in an (M+1)$^+$ peak. To get the ratio of (M+1)$^+$/M$^+$, we need to add all three probabilities:

\[
4.32 + 0.075 + 0.08 = 4.475 = \text{(M+1)$^+$ molecules per 100 M$^+$ molecules}
\]

We can say then that the (M+1)$^+$ peak is 4.475% as high as the M$^+$ peak.

A similar analysis can be easily repeated for (M+2)$^+$:
1Br * 98 = 98 = molecules with an $^81\text{Br}$ molecule per 100 molecules

2O * 0.2 = 0.4 = molecules with an $^{18}\text{O}$ molecule per 100 molecules

$98 + 0.4 = 98.4 = (M+2)^+$ molecules per 100 $M^+$ molecules

The $(M + 2)^+$ peak is therefore 98.4% as tall as the $M^+$ peak.

This method is useful because using isotopic differences, it is possible to differentiate two molecules of identical mass numbers.

References


Outside Links

  - This wikipedia page is about the Mass Spectrometer instrument.

  - This wikipedia page is more directly related to isotope effects, as it focuses on reading mass spectra.

- [http://www.chem.uoa.gr/applets/AppletMS/Appl_Ms2.html](http://www.chem.uoa.gr/applets/AppletMS/Appl_Ms2.html)
  - This applett is fun to play with. It generates isotope peaks in a specified mass fragment.

Problems

1. Predict the $(M+1)^+$ relative peak heights for meta-nitrobenzene.

2. Why would this method of looking at isotope ratios relating to peak heights make distinguishing molecules with Chlorine and Bromine from other molecules very easy?

3. Predict the $(M+4)^+$ relative peak heights for $C_3H_2SCl_2$

4. Predict the $(M+1)^+$ and $(M+2)^+$ relative peak heights for 1,1,1-tribromo-2-propene

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