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:

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

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

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

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

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:

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

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)$^+$:
\[ 1\text{Br} \times 98 = 98 = \text{molecules with an } ^{81}\text{Br molecule per 100 molecules} \]

\[ 2\text{O} \times 0.2 = 0.4 = \text{molecules with an } ^{18}\text{O molecule per 100 molecules} \]

\[ 98 + 0.4 = 98.4 = (M+2)^+ \text{ molecules per 100 M}^+ \text{ molecules} \]

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.

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**References**


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**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.

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**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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