Figure 1 and the isotope abundance data from Table 1, we can see that there are 1.08 $^{13}$C atoms for every 100 $^{12}$C atoms, and the $^{13}$C peak will be 1.08% as large as the $^{12}$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: $^{13}$C, $^2$H, $^{81}$Br, $^{17}$O, and $^{18}$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 $^{81}$Br and $^{18}$O would both increase M by 2, they can be ignored (the most abundant isotopes for Br and O are $^{79}$Br and $^{16}$O). Like the previous example, there are 1.08 $^{13}$C atoms for every 100 $^{12}$C atoms. However, there are 4 carbon atoms in our molecule, and any one of them being a $^{13}$C atom would result in a molecule with mass (M+1). So it is necessary to multiply the probability of an atom being a $^{13}$C atom by the number of C atoms in the molecule. Therefore, we have:

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

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

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

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

Any of the three isotopes, $^{13}$C, $^2$H, or $^{17}$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 $^{81}$Br molecule per 100 molecules

$2O * 0.2 = 0.4 = $ molecules with an $^{18}$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.

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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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