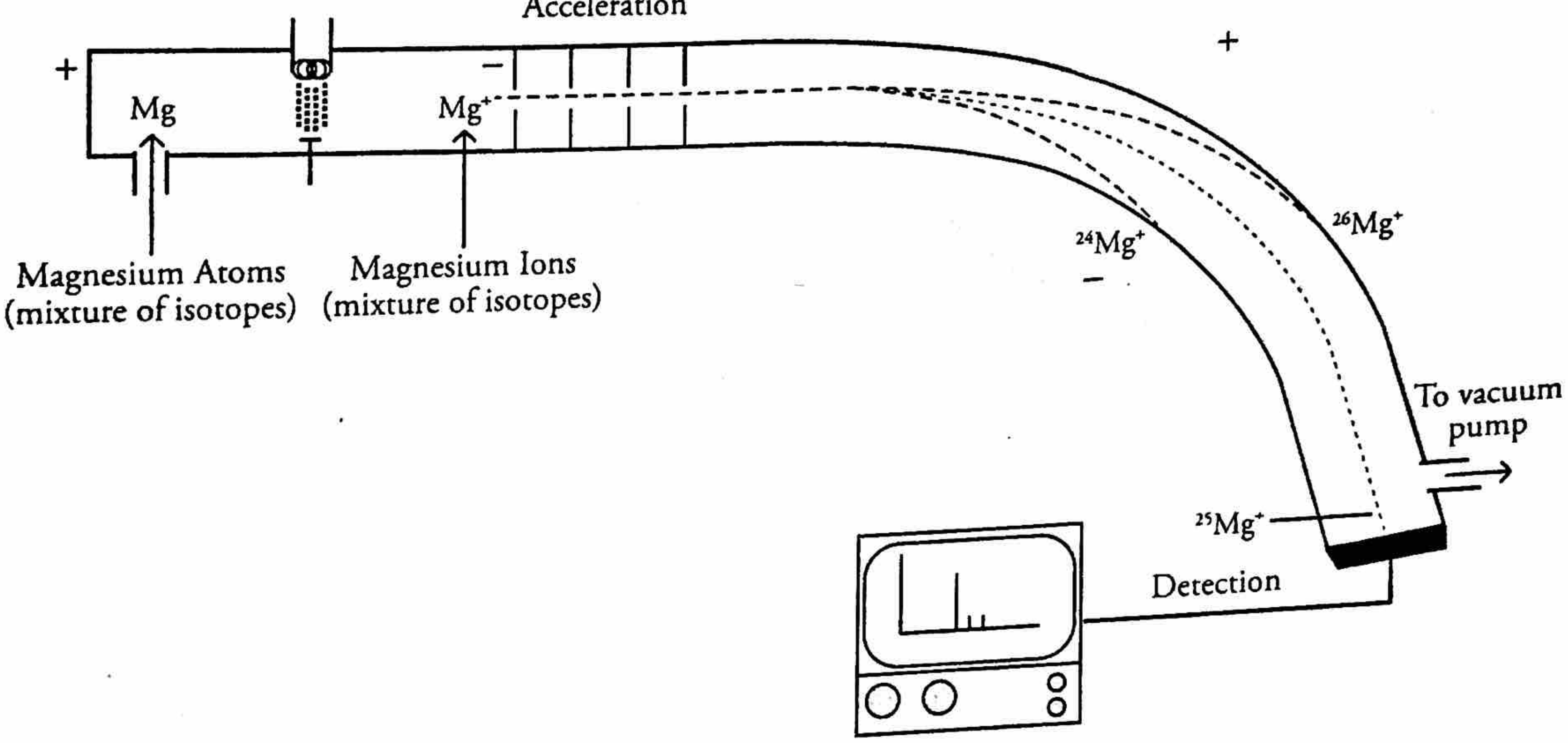
Mass Spectroscopy

How do we know isotopes exist?

Why?

When John Dalton proposed the first formal atomic theory, he stated "Atoms of the same element are identical." Today we know that is not true—many elements contain several different isotopes, or atoms that differ in mass. Mass spectroscopy is the principle technique used to study isotopes. It is used to both "count" and "weigh" atoms in a sample, just not in the traditional sense.

Model 1 – Sorting by Mass



1. According to Model 1 what four processes occur inside a mass spectrometer?
   Ionization, acceleration, deflection, detection

2. Consider where the sample is introduced into the mass spectrometer in Model 1. Which one of the four processes from Question 1 is the first process?
   ionizations

3. Match the four processes from Question 1 to the following descriptions.
   - Detection — Ions collide with a metal plate. Electrons are transferred from the metal to the ion, producing a current and thus a signal to a computer.
   - Deflection — Ions are attracted to the negative side of an electromagnetic field causing separation of the mixture based on mass and charge.
   - ionization — Electrons are knocked off sample particles to form (mostly) +1 ions.
   - acceleration — Ions move through a series of charged plates to form a narrow beam of high speed particles with equal kinetic energy.

4. When a sample is injected into the mass spectrometer, do the atoms or molecules turn into positive or negative ions? Justify your answer with at least two pieces of evidence from Model 1.

positive
→ it has a (+) charge, deflects towards negative beam
→ electromagnetic field

5. According to Model 1, what causes the sample mixture to become separated?

Deflection based on mass and charge

Read This!

The key to mass spectrometry is that all of the particles go into the deflection chamber with the same kinetic energy. They do not, however, have the same **mass/charge ratio (m/z)**. Although most of the ions formed are +1 ions, their masses are different. Therefore, the amount of deflection they experience by the electromagnet is different. The strength of the electromagnet can be varied so only particles with a particular mass/charge ratio can make it to the detector. Other particles collide with the metallic sides of the instrument, are neutralized, and then removed by the vacuum pump. The machine is calibrated using carbon-12 isotopes which are, by definition, exactly 12 amu (12.0000000...amu).

6. Consider the following ions formed in a mass spectrometer. Rank the ions in terms of their degree of deflection by the electromagnet from least to greatest. Greater deflection means a tighter turn towards the negative pole of the electromagnet. Make sure all group members are able to explain the ranking.

$^{19}F^{1+}$	$^{16}O^{1+}$	$^{17}O^{1+}$
1 least	3 most	2

7. Why is it necessary to have the mass spectrometer chamber under vacuum (very low pressure) for it to work properly?

less particles to collide with

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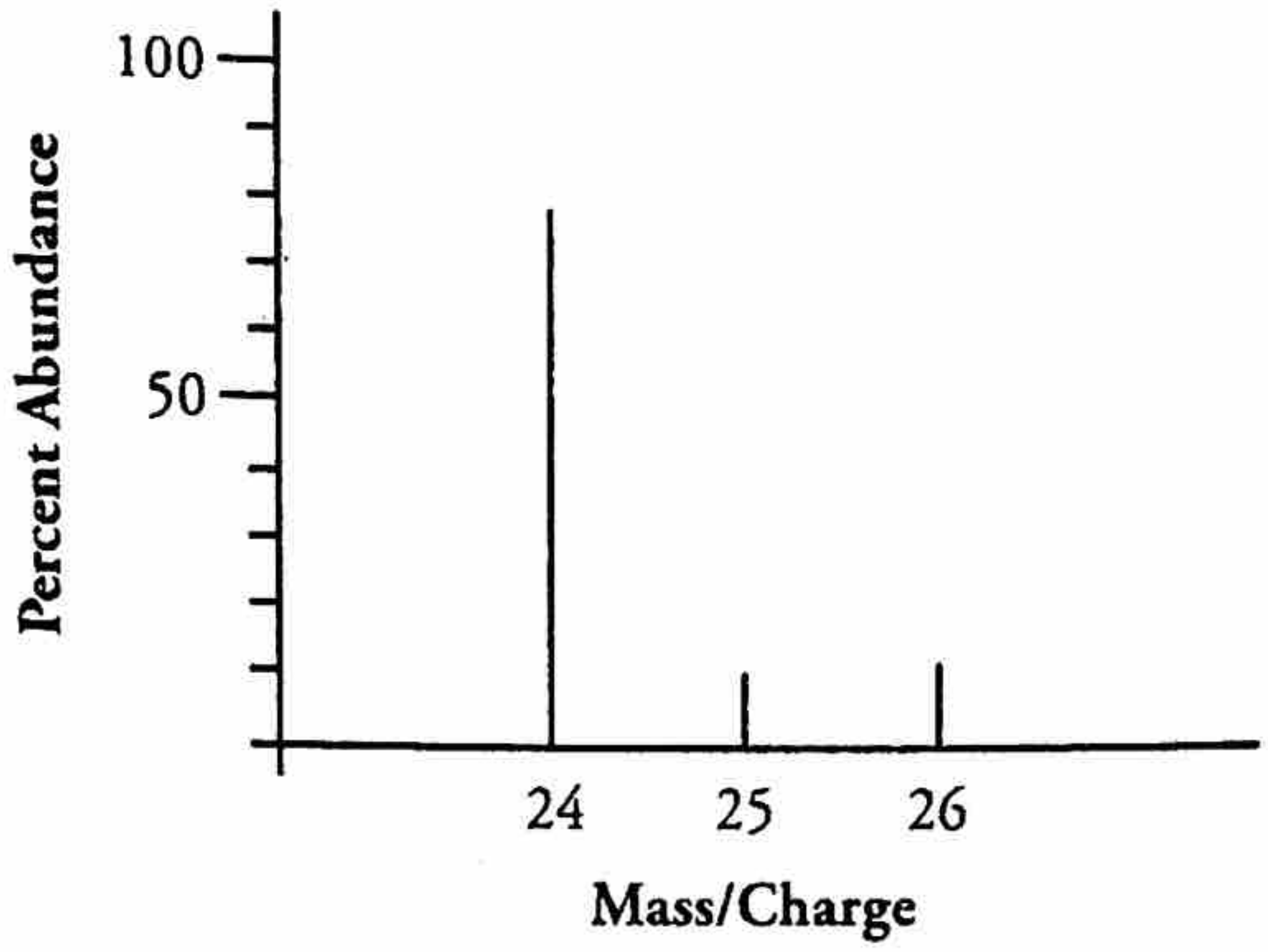
Model 2 – A Mass Spectrum



8. Model 2 is the mass spectrum that resulted from the experiment in Model 1.

   a. What is the mass number of the most common isotope of magnesium?

   24

   b. What is the percent abundance of the most common isotope of magnesium?

   80%

9. The average atomic mass of an element can be estimated from data on a mass spectrum.

   a. Calculate the average atomic mass of magnesium using data from Model 2. *Hint:* You will not get the correct answer if you add 24, 25 and 26 and divide by 3.

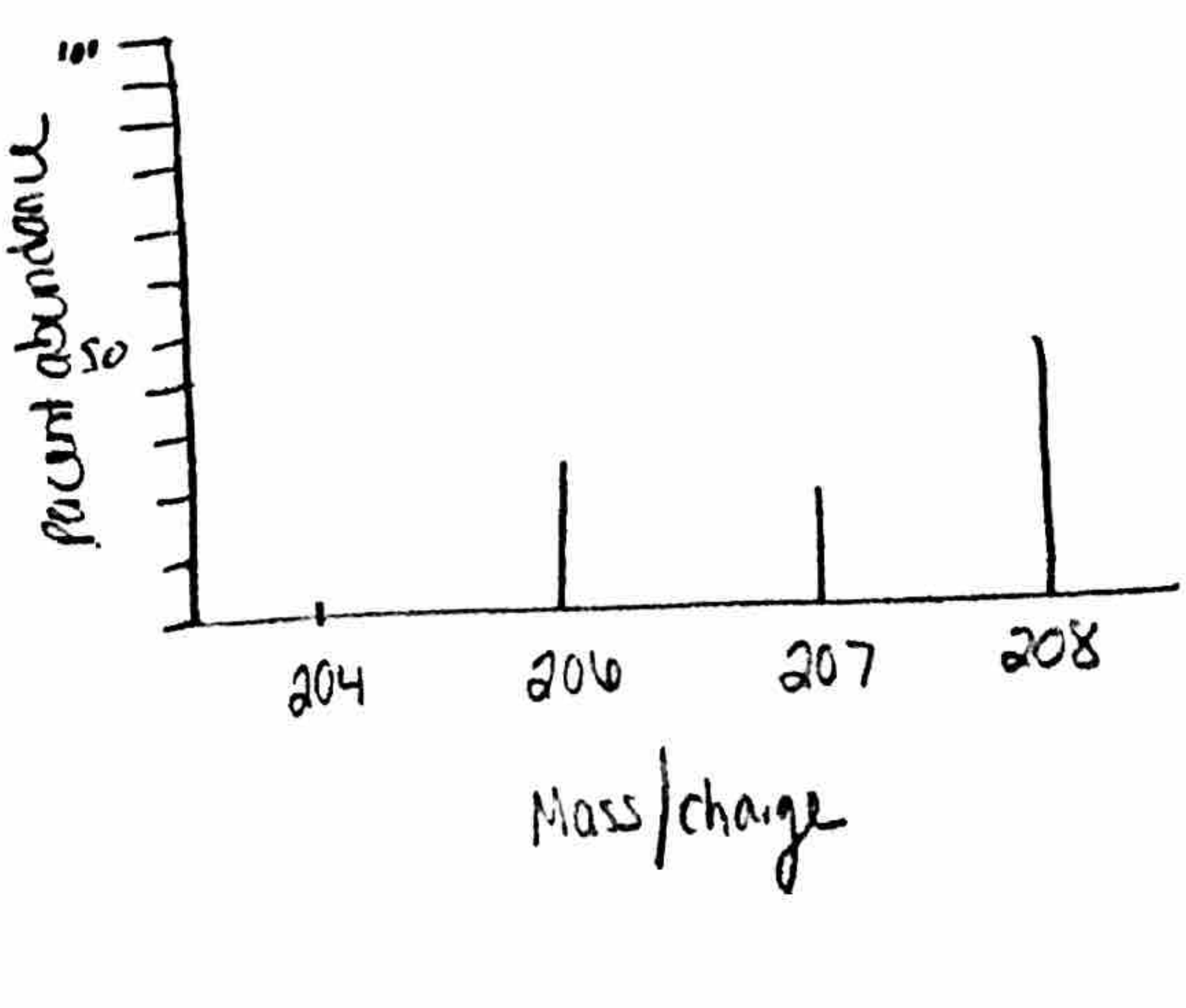
   (24 × .8) + (25 × .1) + (26 × .1) = 24.3 amu

   b. Give two reasons why your calculated value in part *a* is only an estimate of the average atomic mass of the element magnesium.

   - don't know sample size
   - grid lines on chart go by 10's

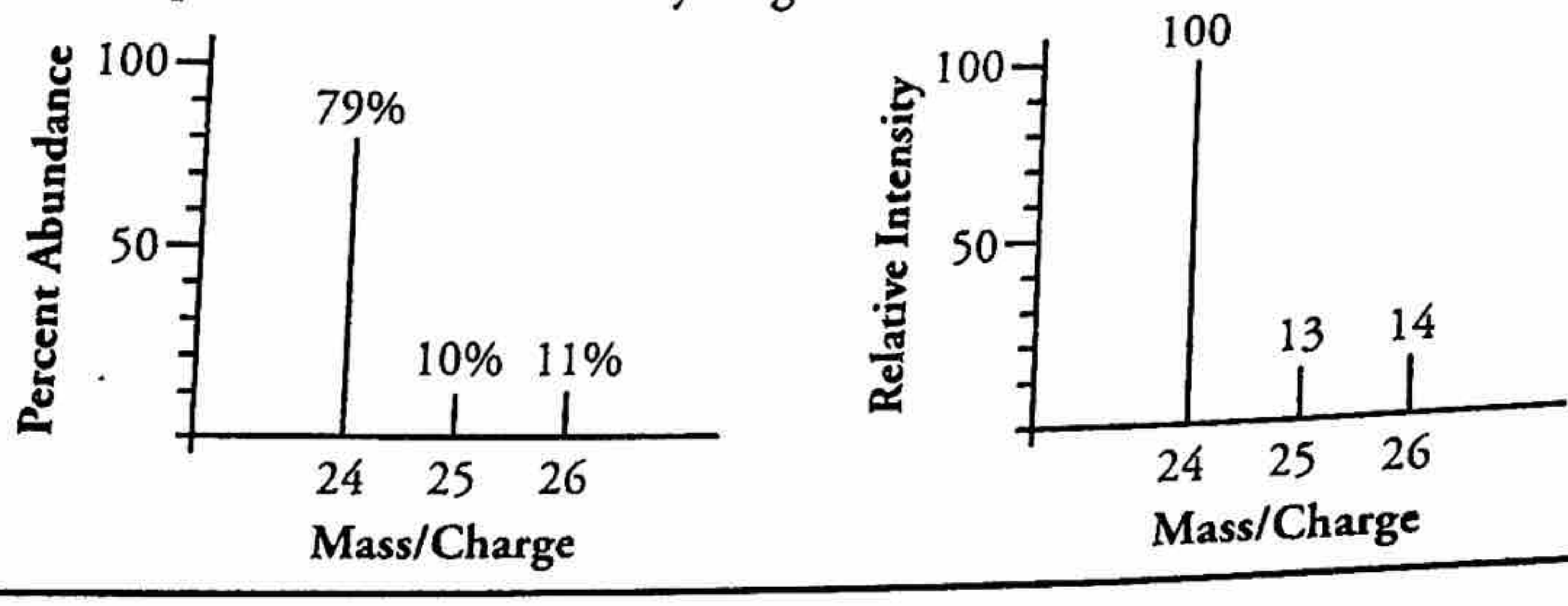
10. The table below provides mass number and percent abundance information for the element lead. Draw a mass spectrum for lead. (You can assume only +1 ions of lead are formed.)

^{204}Pb	1.4%
^{206}Pb	24.1
^{207}Pb	22.1
^{208}Pb	52.4



Read This!

The mass spectra you have been looking at in this activity used percent abundance on the y-axis. Typically, however, the spectra use relative intensity. The ions from the sample are sorted by mass/charge ratio by the mass spectrometer. The ion that hits the detector most often is assigned a relative intensity of 100. The other ions are given proportional relative intensities based on their abundance in the sample. An example of magnesium's mass spectrum shown both ways is given below.



11. Consider the two mass spectra in the *Read This!* box.

   a. The sum of all percent abundances for magnesium is equal to 100. Explain why this is reasonable.

   percentages are always out of 100%.

   b. The sum of all relative intensities for magnesium does not equal 100. Explain why this is reasonable.

   Relative intensities go based of the most abondant species, so that is considered 100%, and the others are relative to the most abundant
   "since tallest peak is assigned 100, then only way there could be 100% is if there is only one isotope)

12. Imagine that the relative intensities on the mass spectra in the *Read This!* box represent the number of particles in a sample.

   a. Theoretically, how many magnesium ions were detected by the mass spectrometer?

   $100 + 13 + 14 = 127$

   b. What percentage of the ions were ^{24}Mg ions? Show mathematical work to support your answer.

   $\frac{100}{127} \times 100 = 79\%$

   c. Show mathematically how a computer might translate the 13 peak in the relative intensity graph to 10% for the percent abundance graph.

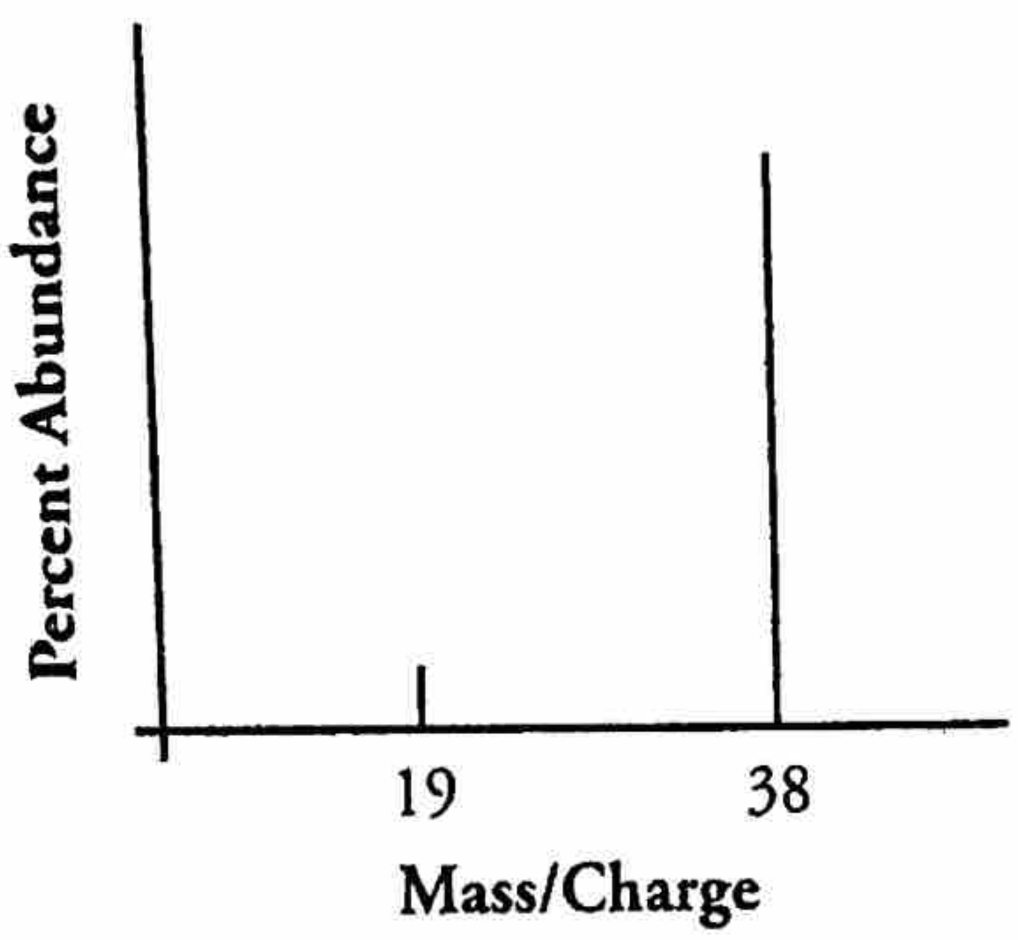
   $\frac{13}{127} \times 100 = 10\%$

STOP

Read This!

The process of ionization inside of a mass spectrometer is quite violent. There are several methods of ionization used in industry, but many of them remove electrons from the atoms or molecules by high energy particle bombardment. In other words, the electrons are knocked off the atoms or molecules by high speed particles colliding with them. Occasionally this process will break apart a molecule. This is called **fragmentation.** The pieces are analyzed by the mass spectrometer along with the whole molecules.

13. The following information was gathered by mass spectroscopy for the element fluorine. Fluorine has only one natural isotope, but it does form diatomic molecules naturally. Propose an explanation for the two lines on fluorine's mass spectrum.



the molecule was not completely ionized, so some of the atoms stayed in molecular form

14. The element chlorine has two natural isotopes: ^{35}Cl (76% abundance) and ^{37}Cl (24% abundance). The mass spectrum of chlorine has five lines.

a. Three of the lines in the mass spectrum are from diatomic molecules of chlorine. List the three possible combinations of the two isotopes and their total mass number.

$^{35}Cl + ^{37}Cl$ ^{37}Cl ^{37}Cl ^{35}Cl ^{35}Cl

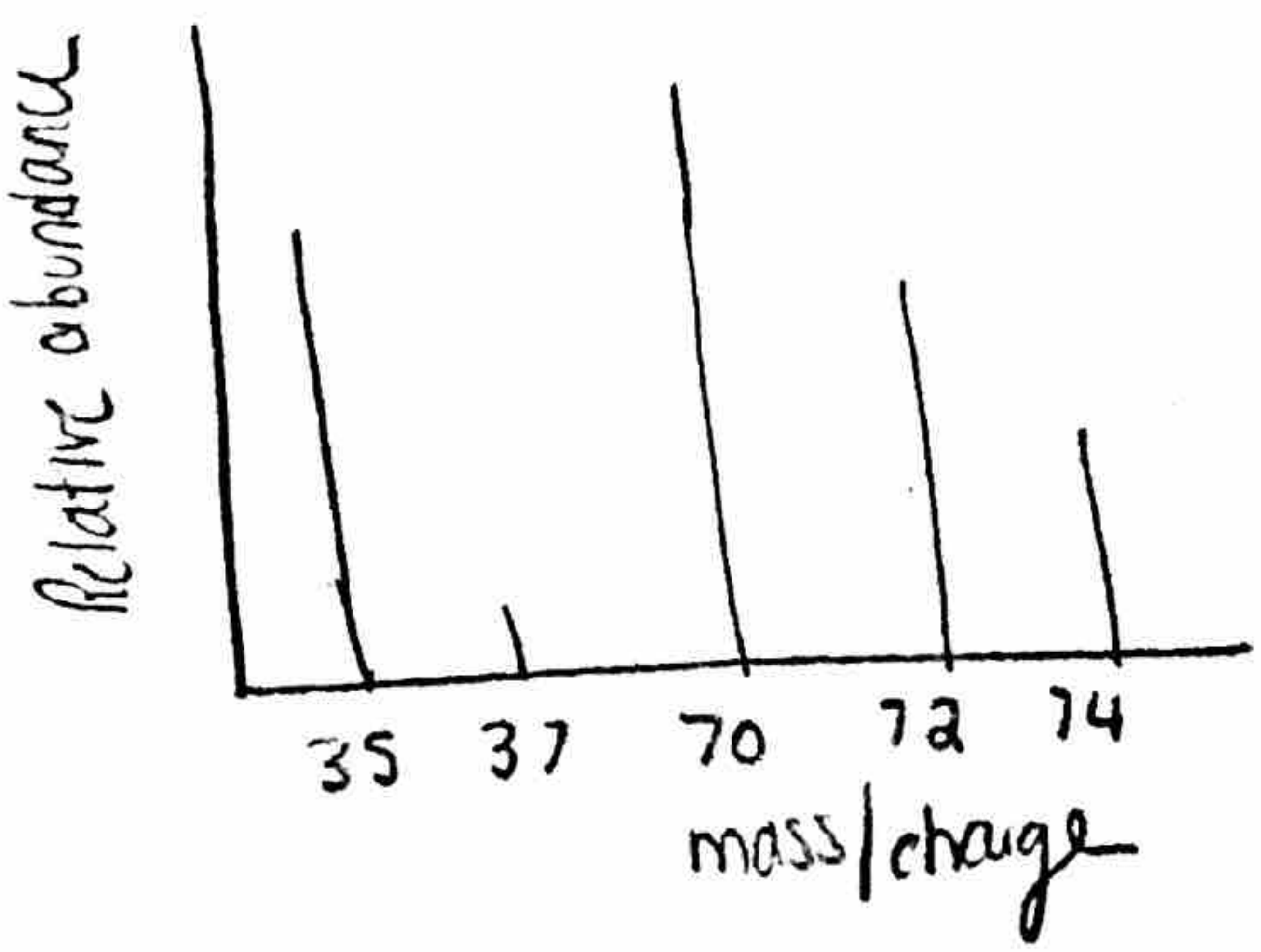
^{72}Cl ^{74}Cl ^{70}Cl

b. Explain the remaining two lines in the spectrum.

35, 37

naturally occuring isotopes

c. Draw a mass spectrum that would result from diatomic chlorine. Include the mass/charge number and estimate the relative abundance of each ion. (Assume only +1 ions are formed.) Although the heights of the peaks are difficult to predict you should be able to determine which will be taller or shorter based on the abundance of each chlorine isotope.



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