A Step-By-Step For Solving Mass Spectroscopy Problems

The problem: m/z = 120 (M; 100%), m/z = 121 (9.8%), and m/z = 122 (.42%)

1. Start by organizing all your data into a chart. This will make it easier to fit the pieces together, and you can be sure you didn't miss anything.

m/z	Molecular Ion	Relative Frequency	So What?
120	M	100%	
121	M + 1	9.8%	
122	M + 2	.42%	

Don't worry, we haven't done any problem solving yet! We just put the information in a chart. Wondering how we were able to get the second column? It's pretty simple. We were told that 120 corresponds with M. So what's 120 + 1? And what's 120 + 2? It's the same as M + 1 and M + 2

2. Okay, everything's organized now. Let's start solving this thing. Now we need to fill in the last column.

m/z	Molecular Ion	Relative Frequency	So What?
120	M	100%	A
121	M + 1	9.8%	B
122	M + 2	.42%	C

Here's what to do with each box:

A: This box will tell you how many Nitrogens are in the formula. You can use the Nitrogen rule; it's super easy and straight forward. If the m/z (the number in the first box) is an even number, there are an even number of Nitrogens in the formula. If it's an odd number, there are an odd number of Nitrogens in the formula. We have an even number (120) so we have an even number of Nitrogens. It's just that simple. But remember, zero counts as an even number too!

B: This box will tell you how many Carbons are in the formula. Just take the relative frequency, in this case 9.8%, and divide by 1.1. The number you get will be the number of Carbons. So with a little bit of math, we divide 9.8 by 1.1 and get 8.9. We're going to round and say there are 9 Carbons in the formula. Be careful though! Dividing by 1.1 is NOT the same as dividing by 1, so yes, you actually need to do the math. I know, long division. And be careful of rounding too. If you get a number that could be rounded either way, it's best to put them both in the box with a question mark. Don't worry about having two answers there—we're getting to that later.

C: This box tells you if there are any Sulfur, Chlorine, or Bromine ions present. Here's an easy way to tell:

If the Relative Frequency Is…	Then this atom is present
~4%	Sulfur
~33%	Chlorine
~100%	Bromine

Okay, so let's look at our relative frequency. 0.42%? That's really small. So we can conclude that there is no Sulfur, Chlorine, or Bromine present in this molecule.

Now we have all our information, and our chart should look something like this:

m/z	Molecular Ion	Relative Frequency	So What?
120	M	100%	Even number of Nitrogens in formula
121	M + 1	9.8%	9 Carbons in formula
122	M + 2	.42%	No Sulfur, Chlorine, or Bromine present

3. Okay, so we have our pretty little chart filled out. Now what? Well, here's where it gets a little math-y. Don't worry, we'll take it step by step. Our m/z is 120, which means the atomic mass of the compound must add up to 120. But where do all those grams come from? Well, there aren't any Sulfur, Chlorine, or Bromine, so we know their molecular weight didn't contribute to that 120. So now where do we go? Well, what's the one element we're sure of right now? Good old reliable Carbon! It never lets us down. There are 9 Carbons in the formula, and each Carbon weighs 12 grams. So let's do a little math here:

   120 grams - (12 grams X 9 Carbons) = 12 grams

   So we have 108 grams accounted for, and 12 grams that came from…hmmm…where *did* they come from? Well, let's figure this out with yet another handy dandy chart.

4.

Oxygen	Nitrogen	12-Oxygen-Nitrogen=Hydrogen	Formula	And the Verdict Is…

Now, I know what you're thinking. How where did these Oxygens and Nitrogens come from? And the Hydrogens? Well, at the end of the day, if it's not Carbon, Sulfur, Chlorine, or Bromine, it'll be Nitrogen or Oxygen. And when that's all figured out, everything left over will be Hydrogen.

So let's start filling this thing out. We only have 12 grams left to find. But wait, what's Oxygen's molecular weight? 16 grams. And what's Nitrogen's molecular weight? 14 grams. Now, I'm no math expert, but something tells me that if you only have 12 grams left, there can't be any Oxygen or Nitrogen in the formula. Let's jump back to step 2 for a minute. Remember when the Nitrogen rule told us there was an even number of Nitrogens in the formula? Well, zero counts as an even number. So everything works out, and the rule fits. Don't you just love when that happens?

Oxygen	Nitrogen	12-Oxygen-Nitrogen=Hydrogen	Formula	And the Verdict Is…
0	0	12 – 0 – 0 = 12	C_9H_{12}	Acceptable
1	0	12 - 16 - 0 = -4	Not Possible	Nope
0	2	12 – 0 – 28 = -16	Not Possible	Nope

Well, you see how the possibilities could go on forever, but there's really only one formula that's going to get that oh so wonderful green "acceptable" that we love so much. So it looks like we've found our formula—there's only one viable option.

Final Answer: C_9H_{12}

And solving mass spec problems is just that easy!