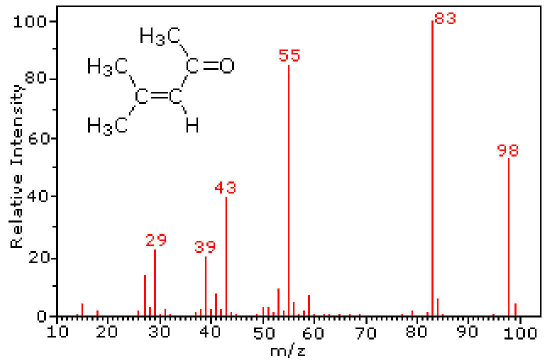
Mass Spectrometry (or MS) is a type of analysis which can give very extensive information about the structure of a molecule, but only for an advanced student. For students in Chem 124, there are a few quick (but useful) bits of information that can be easily learned about a molecule.



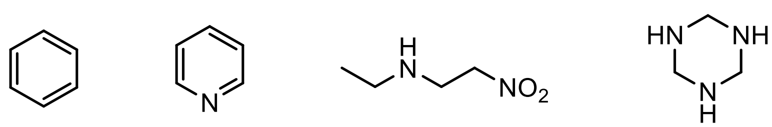
Background

1. In Mass Spectrometry, a neutral molecule is bombarded with electrons, causing the molecule to become positively charged. This charged molecule (the *Molecular Ion*) can then shatter into smaller pieces (*Fragment Ions*). All of these ions are then pulled into an analyzer, which then produces data on the weight and abundance of the various ions produced.
2. Mass Spectral data is shown as a graph, where the vertical axis gives abundance, and the horizontal axis gives the mass to charge ratio (m/z).
    a. Abundance or Relative Intensity: taller peaks = more ions found, smaller peaks = fewer ions found.
    b. Mass to Charge ratio (m/z): usually, a molecule only gets ionized one time, creating a single charge (+1) on the ion. Therefore, if the charge is 1, then the value of the m/z really corresponds to the mass. Ex: a peak at m/z = 147 means that it came from an ion which weighs 147 amu and has a charge of +1 (m/z = 147 / +1)
3. Although many peaks can be seen in a Mass Spectrum, you should focus your attention on the peak or group of peaks farthest to the right. These peaks will represent the largest masses, and are therefore most likely to be the molecular ion.

Analysis

At this level, you should always focus analysis on the molecular ion. Please note that there are often tiny peaks on the Mass Spectrum; they should generally be ignored (see exception for isotope effects below). There are three basic bits of information to be gained from MS:

1. **Molecular Mass**: The largest peak which is farthest to the right in the mass spectrum is usually the Molecular Ion. (see exceptions for isotope peaks below). What would be the Molecular weight for the compound in the MS above?
2. **Odd or Even Number of Nitrogen atoms in the Molecule**: Once you have found the molecular ion, check to see if its molecular weight is odd or even. If the mass is even, then there will be an even number of Nitrogen atoms in the molecule (e.g. 0,2,4,6, etc.) If the mass is odd, then there will be an odd number of Nitrogen atoms in the molecule (e.g. 1,3,5, etc) Practice to prove to yourself that this is correct. What are the molecular weights of each molecule on the next page? Do the odd MW molecules have an odd number of N's? Do the even MW molecules have and even number of N's? (Note: when calculating molecular weight for MS, use only real, whole-number values for the weight of each atom—do not use the averages printed on a periodic table.)

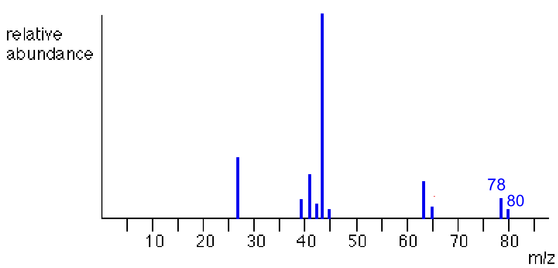


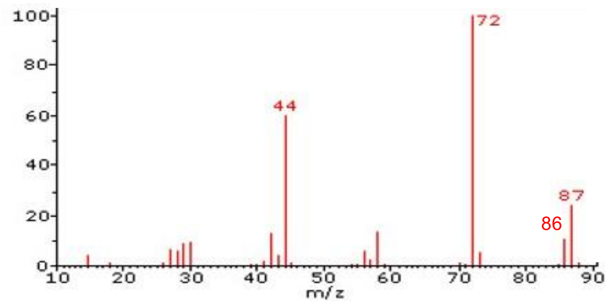
Atom	Mass	Atom	Mass
H	1	N	14
C	12	O	16

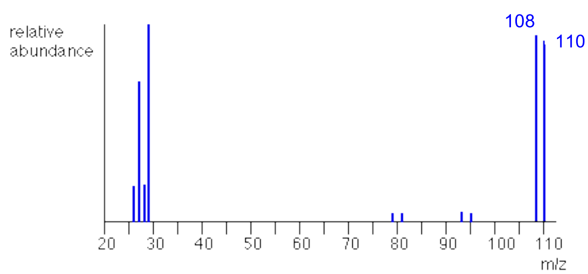
3. **Isotopes**: As stated above, you need to use real weights, not average weights to calculate masses for MS data. Most atoms have only one dominant isotope, so their mass is pretty much what you would expect (see table above). However, some atoms have isotopes with very different masses, and both are quite abundant. Two atoms that exhibit these properties are Bromine and Chlorine (see below).

Atom	Mass	Relative Abundance	Atom	Mass	Relative Abundance
^{35}Cl	35	3	^{79}Br	79	1
^{37}Cl	37	1	^{81}Br	81	1
Average Mol. Weight		35.5	Average Mol. Weight		79.9

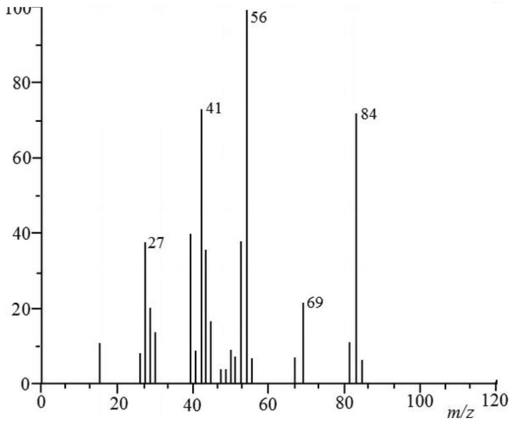
Because of this, molecules that contain either Cl or Br will exhibit 2 peaks for the Molecular Ion, the larger peak for the more abundant ion, and a second, smaller peak for the second isotope. You will recognize the isotope peak because it will be EXACTLY 2 mass units heavier than the molecular ion and will EXACTLY mirror the relative abundance of the second isotope. That means that for Bromine, the two peaks are almost identical in height, while for Chlorine the second peak is 1/3 the size of the first peak. Practice telling if the MS data below show molecules that contain Br, Cl or neither.







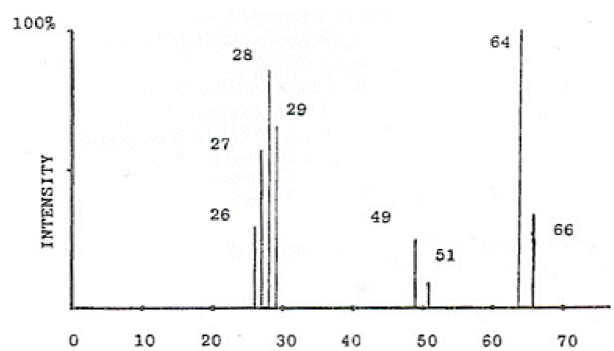
Practice: For each spectrum below, analyze for the three traits: 1) What is the molecular weight? 2) Does the molecule have an odd or even number of N's in it? 3) Does it contain Br? Cl? Finally, pick one of the molecules at the bottom of the page whose structure matches the information from each spectrum.



1) ______________________

2) ______________________

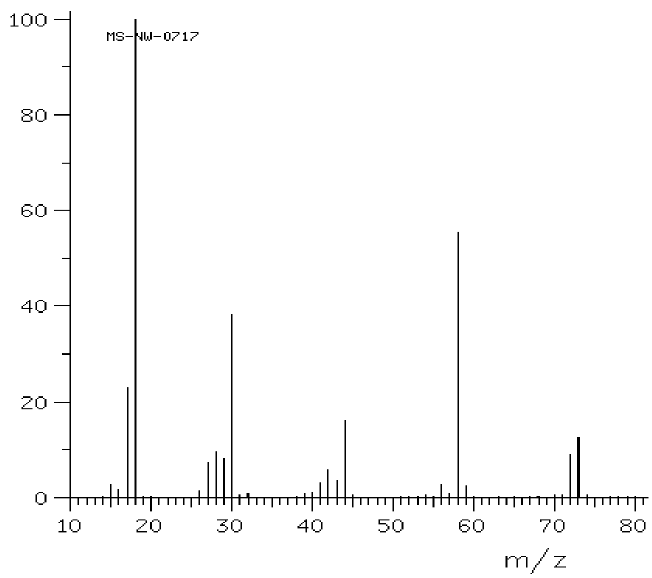
3) ______________________



1) ______________________

2) ______________________

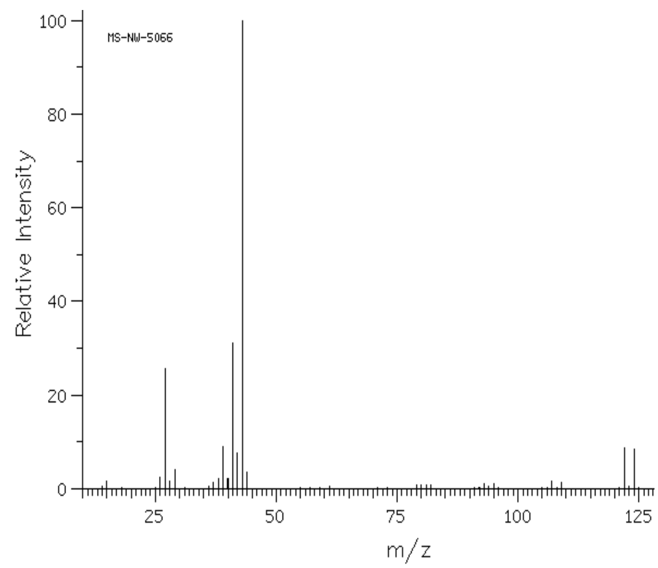
3) ______________________



1) ______________________

2) ______________________

3) ______________________



1) ______________________

2) ______________________

3) ______________________

Possible Compounds