Here are a list of steps to follow when interpreting a mass spectrum. This simplified list will help you to interpret many spectra, however there are other mechanisms of fragmentation which cannot be covered in this brief tutorial.

**Steps to interpret a mass spectrum**

1. Look for the molecular ion peak.
   - This peak (if it appears) will be the highest mass peak in the spectrum, except for isotope peaks.
   - Nominal MW (meaning=rounded off) will be an even number for compounds containing only C, H, O, S, Si.
   - Nominal MW will be an odd number if the compound also contains an odd number of N (1,3,...).

2. Try to calculate the molecular formula:
   - The isotope peaks can be very useful, and are best explained with an example.
     - Carbon 12 has an isotope, carbon 13. Their abundances are \( ^{12}\text{C}=100\% \), \( ^{13}\text{C}=1.1\% \). This means that for every 100 \( ^{12}\text{C} \) atoms there are 1.1 \( ^{13}\text{C} \) atoms.
     - If a compound contains 6 carbons, then each atom has a 1.1\% abundance of \( ^{13}\text{C} \).
     - Therefore, if the molecular ion peak is 100\%, then the isotope peak (1 mass unit higher) would be 6\%\times1.1\%=6.6\%.
     - If the molecular ion peak is not 100\% then you can calculate the relative abundance of the isotope peak to the ion peak. For example, if the molecular ion peak were 34\% and the isotope peak 2.3\%: \( \frac{2.3}{34}\times100 = 6.8\% \). 6.8\% is the relative abundance of the isotope peak to the ion peak. Next, divide the relative abundance by the isotope abundance: \( \frac{6.8}{1.1}=6 \) carbons.
     - Follow this order when looking for information provided by isotopes: (A simplified table of isotopes is provided in the introduction, more detailed tables can be found in chemistry texts.)
       - Look for A+2 elements: O, Si, S, Cl, Br
       - Look for A+1 elements: C, N
       - "A" elements: H, F, P, I

3. Calculate the total number of rings plus double bonds:
   - For the molecular formula: \( \text{C}_x\text{H}_y\text{N}_z\text{O}_n \)
     - \( \text{rings + double bonds} = x - \frac{1}{2}y + \frac{1}{2}z + 1 \)

4. Postulate the molecular structure consistent with abundance and m/z of fragments.
   - More information on specific fragmentation can be found in the quiz for each functional group.

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