CONCEPT: MASS SPECT- COMMON ISOTOPES

Isotopes are often visible on a mass spectrum, due to their differing weights. They can be used for structure determination.

Understanding the (M + 1) Peak

1.1% of all carbon is found as ^{13}C, adding a small but distinctive (M + 1) peak proportional in size to the number of carbons.

- This proportion is fairly consistent, so it gives rise to ***two helpful equations***

1. *Calculating Height of (M + 1)*

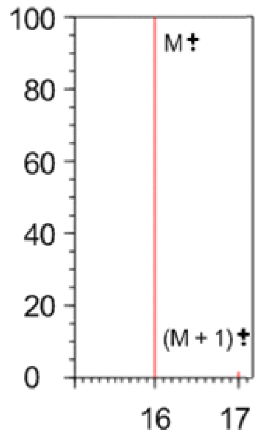
(# carbons x 1.1%)
= (M + 1)$^{+\cdot}$ Height

2. *Calculating Number of Carbons*

$$\frac{(M+1)^{+\cdot}}{M^{+\cdot}} \times \frac{100\%}{1.1\%}$$

≈ # carbon(s)

Methane

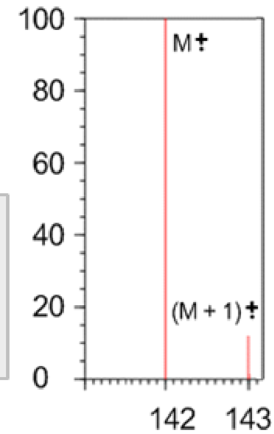


(1 x 1.1%)
= ____%

$$\_\_\_\_ \times \frac{100\%}{1.1\%}$$

≈ ___ **carbon(s)**

Decane



(10 x 1.1%)
= ____%

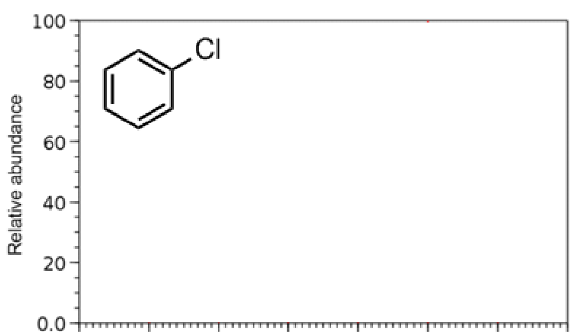
$$\_\_\_\_ \times \frac{100\%}{1.1\%}$$

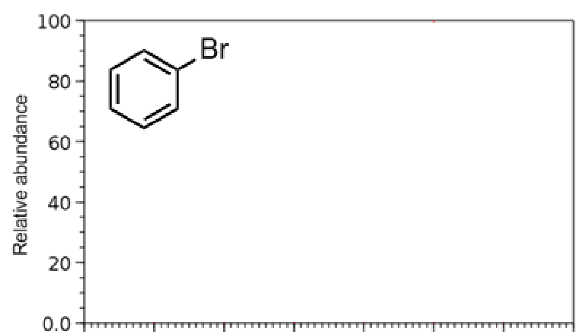
≈ ___ **carbon(s)**

Understanding the (M + 2) Peak

The halogens –Cl and –Br give distinctive (M + 2) peaks due to their unusual patterns of isotopic abundance

- ^{35}Cl = 75.8% and ^{37}Cl = 24.2%, yielding an approximate 3:1 ratio at (M + 2)
- ^{79}Br = 50.7% and ^{81}Br = 49.3%, yielding an approximate 1:1 ratio at (M + 2)

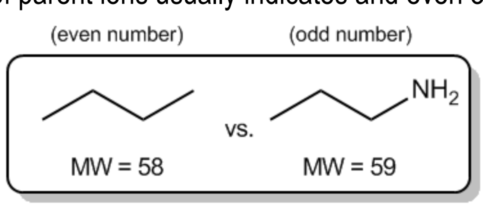




The Nitrogen Rule

Unlike carbon, nitrogen forms 3 bonds. We can use this information to determine the number of nitrogens in a molecule.

- Even or odd molecular weight of parent ions usually indicates and even or odd number of nitrogens present



<u>PRACTICE</u>: Propose the number of carbons for a compound that exhibits the following peak in its mass spectrum:

a. $(M)^{+\bullet}$ at m/z = 72, relative height = 38.3% of base peak
   $(M+1)^{+\bullet}$ at m/z = 73, relative height = 1.7% of base peak

b. Predict the approximate height of the (M + 1) peak for the molecule icosane, molecular formula $C_{20}H_{42}$.

c. Draw the expected isotope pattern that would be observed in the mass spectrum of CH_2Br_2. In other words, predict the relative heights of the peaks at M, (M + 2), and (M + 4) peaks.