Quiz #2 Mass Spec Name _____

Useful Information

$KE = 1/2\ mv^2$ $KE = z\ e\ V$ $F_B = z\ e\ B\ v$ $F_C = m\ v^2 / r$
$V = J / C$ $J = kg\ m^2 / s^2$ $T = kg / s\ C$
$N = 6.022 \times 10^{23}$ $e^- = 1.602 \times 10^{-19}\ C$
atomic masses: $^{12}C = 12.011$ $^{14}N = 14.003$ $^{16}O = 15.995$ $^{1}H = 1.008$
R.P. = m / Δm
Natural abundances: $^{35}Cl = 75.8\%$ $^{37}Cl = 24.2\%$ $^{79}Br = 50.7\%$ $^{81}Br = 49.3\%$

1. (3 pts) What are the 3 **main** parts of an mass spectrometer:

(a)

(b)

(c)

2. (8 pts) Our Agilent GC-MS is able to consistently produce linewidths 0.60 amu (that's the linewidth at half height). PFTBA (perfluorotributylamine, the internal standard we use calibrate and tune our MS) shows major fragments at 69.00, 218.90, and 502.00 amu.

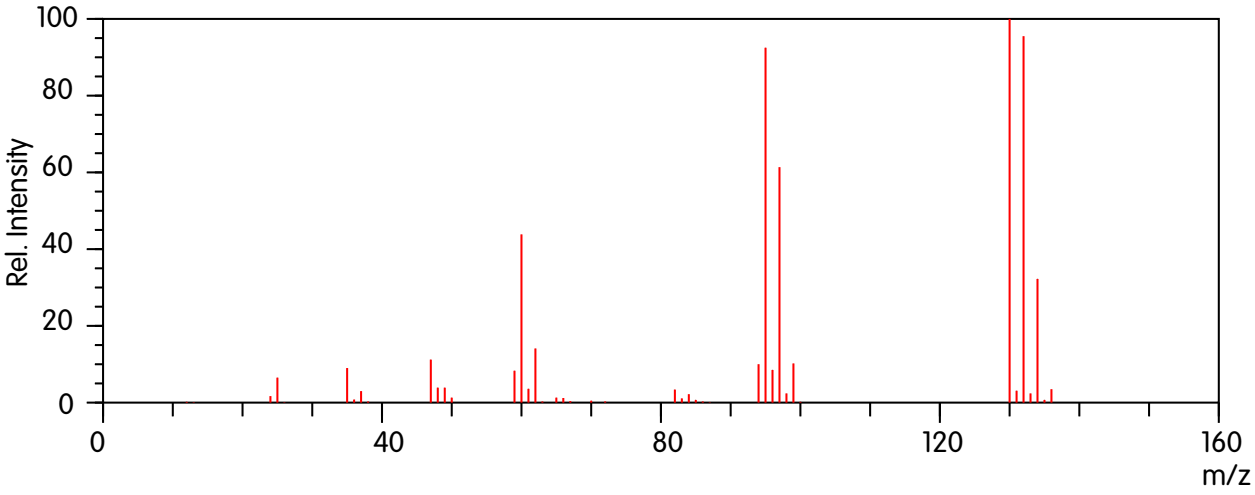
For each of those 3 peaks calculate the resolving power of our instrument.

Is the resolving power constant across the range of masses?

3. (15 pts) This past fall (2019) I was working with organic students to help them identify unknowns using GC-MS. In addition to their unknown peaks, *every* GC trace showed a peak at about 3.5 minutes. I got annoyed because it looked like the organic students had (yet again) contaminated the CH_2Cl_2 bottle used to prep samples.

So I asked Suchen to put out a fresh bottle of CH_2Cl_2. Then I discovered that it too had this same contaminant. I then checked the original bottle of CH_2Cl_2. It too was contaminated. I concluded the material we had purchased had not been well purified.

Determine what the contaminant was based on the mass spec below.



(a) What are the masses of the parent peak?

(b) What atom/isotope is indicated by the number of parent peaks?

(c) Consider the peaks of the fragment at 95, 97, and 99 amu. What isotopes (how many and what kind) are present in each of those 3 peaks? Be specific.

(d) For the fragment at 95-99 amu, calculate the theoretical peak heights based on the abundances of those isotopes given on page 1.

(e) What is the molecular formula of the fragment at 95-99 amu?

(f) What is the molecular formula of the fragment at 60 / 62 amu?

(g) What is the structure of the contaminant?

4. (8 pts) (a) Draw a schematic picture of a quadrupole mass selector.

(b) Describe how a quad MS works. How does it separate ions?

5. (12 pts) In chemical ionization mass spectrometer (CI MS) a reagent gas is mixed with the analyte.

(a) What reagent gas is commonly used in this method?

(b) When the reagent gas is bombarded with high energy electrons, it creates a plasma of cations. List 3 of the cations formed under these conditions and give a chemical equations that shows how they are formed.

1.

2.

3.

(c) Give two examples of what analyte cation is formed when it reacts with two specific plasma cations.

1.

2.

6. (5 bonus points) (a) Draw a schematic picture of the MS detector used in our MS.

(b) What material coats the inside of the dynode in the MS detector?