Chapter 11 Solutions

1. The main MS detectors used with ICP sources are quadrupole and magnetic sector analyzers.

5. The system is shown in Figure 11-10. The interface is called a skimmer, which blows ions out of the torch stream (the sampling cone) into the mass analyzer.

8. The internal standard can be used to quantify substances. It is assumed that the detector response is linear for all masses (and is linear). If that is the case, then the peak height (or peak area) of the internal standard will be directly proportional to the concentration of the standard. The ratio of peak heaights will be the same as the ratio of the concentration of the standard to the concentration of the analyte.

11. In the case of a tandem mass spec, the secondary ion-MS would refer to the second (harder) MS source. In that case, the secondary source gives fragmentation patterns (because the primary source would be soft and mainly give the molecular ion). These fragmentation patterns generally give information about functional groups on the analyte molecule

Chapter 20 Solutions

2. Electron impact is harder than field ionization, therefore would get more information about functional groups with the former, at the potental cost of losing the molecular ion; the latter would ensure that the molecular ion survived so that the overall molecular formula could be confidently assigned. Chemical ionization is generally put as an intermediate level between these two, but also has the complication of potentially adding functional groups to the molecular ion (for example, if CH4 was the carrier gas, an H^+ or a CH_3^+ might be added to the molecular ion).

5. Recall that the formula is $m/z = B^2r^2e/2V$, or $m/z = cB^2/V$, where "c" is a constant taking into account the (constant) radius, the elementary charge, and the 2.
If 0.126 T and 3.00×10^3 V focusses CH_4^+ (m/z = 16 amu), then "c" = 16*3000/0.126 = 3.81×10^5.
(a) range would be 0.126 to 0.498 T.
(b) range would be 3000 to 192 V.

10. For two peaks that are just resolved, $R_s = m/\Delta m$ (use average mass for m)
(a) Rs = 28.0124/0.0126 = 2.22×10^3
(b) Rs = 28.0131/0.0364 = 770
(c) Rs = 85.06487/ = 7.09×10^3
(d) Rs = 174/116 = 1.5

11. (a) If ^{79}Br:^{81}Br is exactly 1:1, the $(M+2)^+$ peak would be exactly 2x larger than the M^+ peak (or $(M+2)^+ : M^+$ is 2:1)
(b) The 4 options are M^+ ^{35}Cl&^{79}Br (0.76*0.5 = 38%), $(M+2)^+$ ^{35}Cl&^{81}Br (0.76*0.5 = 38%), $(M+2)^+$ again ^{37}Cl&^{79}Br (0.24*0.5 = 12%), and $(M+4)^+$ ^{37}Cl&^{81}Br (12%). Therefore, the $(M+2)^+ : M^+$ would be 50:38 (or 1.3:1)
(c) The four options are 35/35 (0.76*0.76 = 58%), 35/37 (0.76*0.24 = 18%), 37/35 (18%), and 37/37 (6%). Total (M+2)+ peak intensity is 18+18, or $(M+2)^+ : M^+$ would be 58:36 (or 1.6:1)

15. The peaks are assigned as follows:

<u>*m/z*</u>	<u>ID</u>
117, 119, 121	CCl_3^+ (117 has no ^{37}Cl, 119 has one ^{37}Cl, 121 has two ^{37}Cl)
131, 133, 135	$C_2H_2Cl_3^+$ (same distribution with the ^{37}Cl)

This is assuming the peak with three 37Cl (at 0.24^3 is lost in the noise)

16. The M+ peak will have the most common abundancies of C, H, and Cl (^{12}C, ^{1}H, and ^{35}Cl).
Thus, the $(M+1)^+$ peak must be $^{13}CH_2Cl_2$ and $C^2H^1HCl_2$.
The $(M+2)^+$ peak is mostly $CH_2{}^{35}Cl^{37}Cl$.
The $(M+3)^+$ peak is mostly $^{13}CH_2{}^{35}Cl^{37}Cl$.
The $(M+4)^+$ peak is mostly $CH_2{}^{37}Cl_2$.