CHEMISTRY 133 – Spring, 2016
Quiz 6 – Solutions

1. A halogenated hydrocarbon is analyzed by mass spectrometry with a parent ion observed with a mass to charge ratio of 238. Fragmentation indicate that it has at least one Br atom and one Cl atom (seen by loss of 35 and 79). Given the ratio of M + 2/M, M + 4/M and M + 6/M (below), **determine the number of Br and Cl atoms** assuming no other isotopes contribute significantly to these peaks. There is no observable peak at the M + 8/M location. The relative abundances of these isotopes are $^{37}Cl/^{35}Cl$ = 32/100 and $^{81}Br/^{79}Br$ = 97/100. Explain your answer. (10 pts)

Observed ratios	M + 2/M	M + 4/M	M + 6/M
	160.2/100	72.1/100	9.9/100

The M+2/M, M+4/M, and M+6/M are intensity ratios. The lack of an M+8/M peak means there are at most 3 halogens (as 4 halogens would give rise to a small M+8 peak due to all heavy isotopes). We also know we don't have 3 Br's as this gives a mass of 237. Thus possibilities are 3 Cl's, 2 Cl's and 1 Br, or 1 Cl and 2 Br's.
We then can calculate M+2/M ratios for each of these:
3 Cls: M+2/M = 3(32/100) = 96/100 (too small)*
2 Cl's and 1 Br *M+2/M = 2*(32/100) + 97/100 = 161/100 (2 in front of Cl ratio because either Cl can be ^{37}Cl)*
1 Cl and 2 Br's M+2/M = 2(97/100) + 32 = 226/100 (too big)*

Bonus Question (2 pts). Show the calculation which will give expected ratios for either M + 4/M or M + 6/M based on your answer above.
M+4/M: this requires 2 ^{37}Cl or 1 ^{37}Cl and 1 ^{81}Br.
(32)(32)/[(100)(100)] + (2)(32)(97)/[(100)(100)] = ***72.3/100***
M+6/M: this requires all M+2 isotopes: (32)(32)(97)/[(100)(100)(100)] = (99,328/10000)/100 = ***9.93/100***