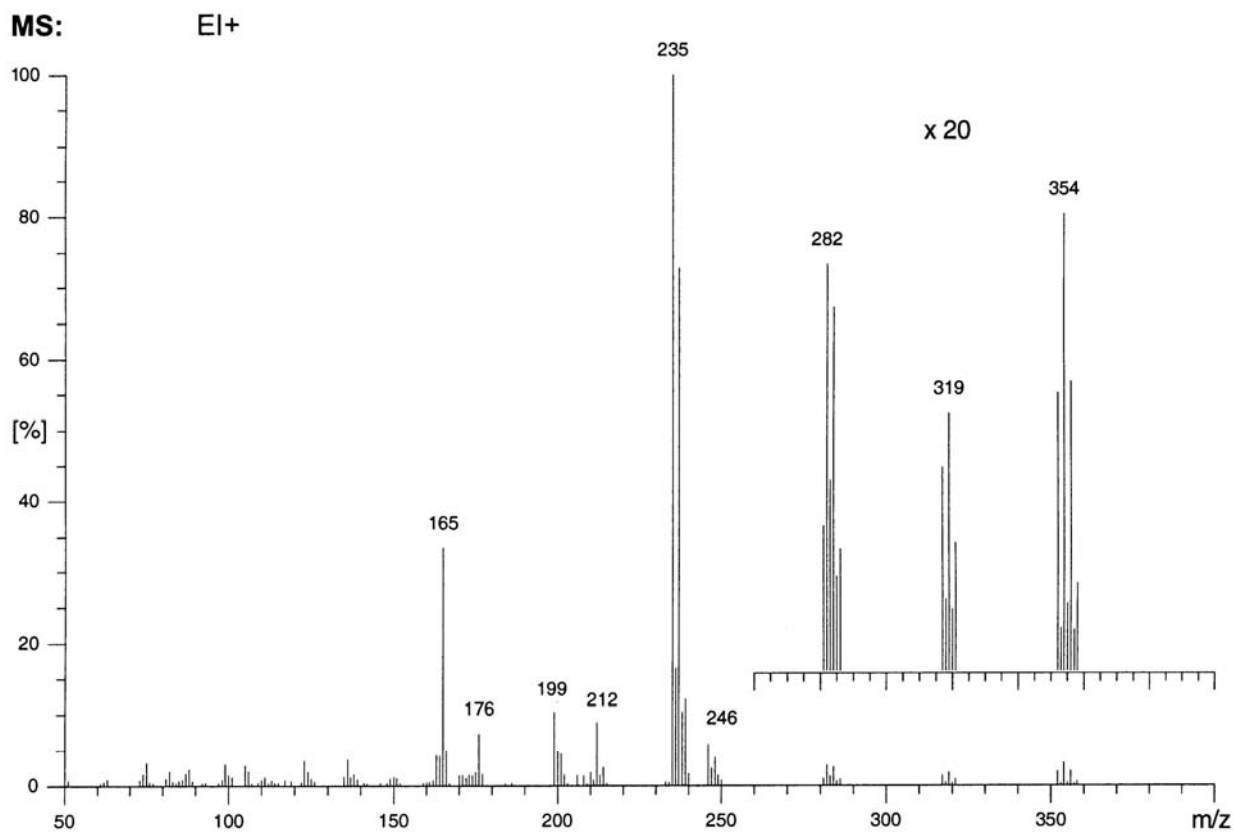


In-Class Exercise: Halogen Isotope Patterns

The spectrum below is an electron-ionization (EI) MS of DDT, the famously banned, chlorinated aromatic insecticide. (Can't tell you what DDT stands for—it would give away the answer to the problem.) DDT contains only C, H, and Cl atoms.



- The set of peaks at $m/z = 354$ corresponds to the ionized parent. Based on the pattern of peaks at this mass, what do you guess is the molecular formula of DDT? (*Hint:* For $C_xH_yCl_z$, what is the probability that there will be z ^{35}Cl 's and no ^{37}Cl 's? What is the probability that there will be no ^{35}Cl 's and z ^{37}Cl 's?)
- The highest-mass daughter fragments at $m/z = 319$, 282, and 235 correspond to sequential losses of at least a Cl atom. What is lost with each fragmentation, and do the resulting isotope patterns match your predictions?