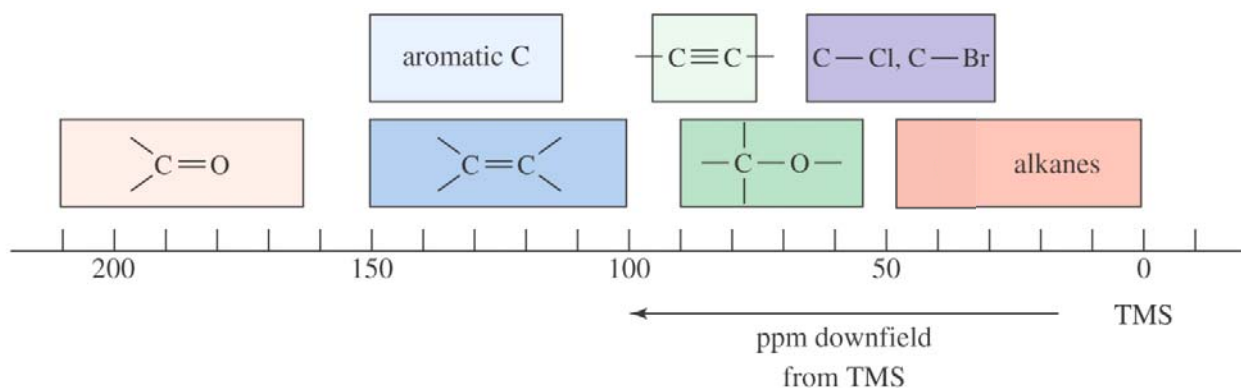**In-Class Exercise Solutions:**
**$^{13}$C NMR Spectroscopy**

a. Answering this problem really required a $^{13}$C chemical shift table. Here's a condensed one:



The NMR on page 2 has one peak in the carbonyl range, 6 peaks in the aromatic/alkene region, and two alkyl carbon peaks. Given the high degree of unsaturation in the molecular formula, and the convenience of 6 aromatic carbons, we can guess that the molecule is an asymmetric substituted benzene. Looking at the aromatic chemical shift chart in Pretsch, the only substituent that could shift an aromatic peak all the way to $\delta$ = 156 ppm would be one -OH or -OR group. The two alkane protons are too far upfield to be attached to oxygen, so they can't be the R.

Looking at peak intensities, the carbonyl carbon, the aromatic -OH/-OR carbon, and one of the other aromatic carbons are short. We can guess that this means they don't have protons attached (and the resulting slow relaxation times cause the peaks to be shortened). So the aromatic ring has another substituent. That substituent could be the carbonyl, but then we'd have to explain the other oxygen. An easier way would be for the substituent to be -CH₂CH₂COOH:
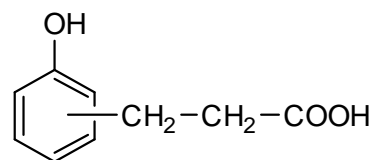


Then the question becomes, is the ring *meta-* or *ortho-* substituted? I'm not sure that you could answer this question. If you run through the math in Pretsch's chemical shift table, either one would be close to explaining the short $\delta$ = 131 ppm peak. The actual answer is *ortho-*, but I'm not sure you could have figured that out from the $^{13}$C NMR alone.
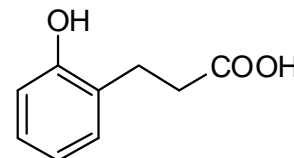
b.  As we discussed in class, even though there are a lot of acetone $^{13}C$ atoms in the NMR sample, they relax very slowly because they have no attached $^1H$ atoms. As a result, in this NMR you don't see them. (If the sample were a bit less concentrated, I bet you would.)

c.  You should see a 1:3:6:7:6:3:1 septet from the -$^{13}CD_3$ groups. This is because each deuterium atom splits the original carbon peak three times in a 1:1:1 ratio.

Acetone-$d_6$