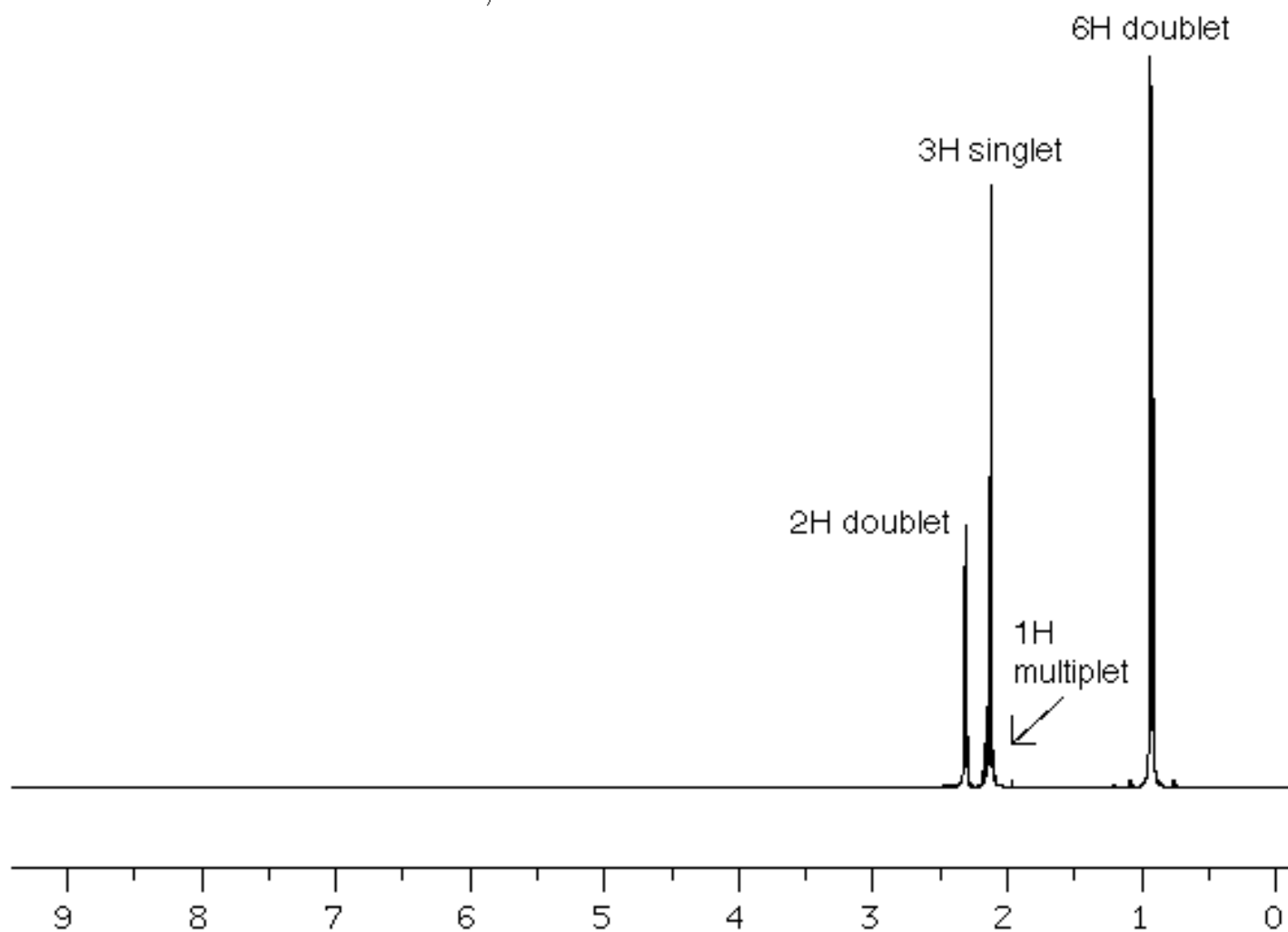
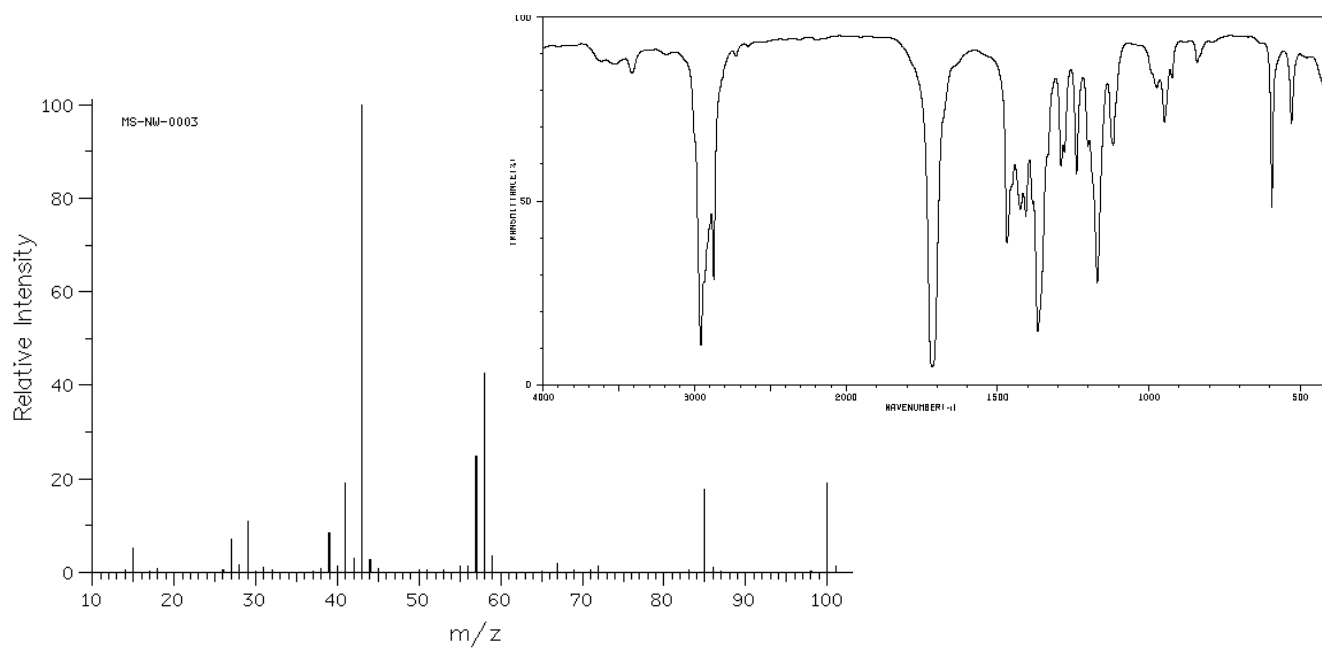


Organic Chemistry II

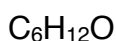
CHM 224

In Class Assignment



Solution Strategy

1. Try to get a molecular formula.
 - a. more than likely, the molecular weight of our unknown is 100 (M^+ seen on the mass spectrum as $m/z = 100$), so let's start with that assumption.
 - b. other than C and H, what other atoms are in our molecule?
 - i. M^+ is even, so even number of nitrogens (probably zero) - and IR confirms
 - ii. IR shows an C=O stretch at about 1700 cm^{-1}
 - iii. Halogens not seen in mass spectrum
 - c. to find molecular formula, assuming only C, H and one O
 - i. Subtract one oxygen from 100 ($100 - 16 = 84$) and add C and H into 84.



This is unlikely a carboxylic acid (which would contain two oxygen atoms) because there is no OH stretch $\sim 3300\text{ cm}^{-1}$. Although one might argue it could still be an ester (which also has two oxygens), however if it were, the number of hydrogens in the resulting molecular formula wouldn't add up to what's seen in the ^1H NMR.

2. Degree of unsaturation = 1

3. Proton NMR:

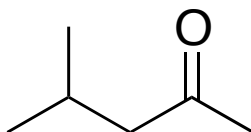
6H d = two equivalent CH_3 groups that are next to a CH

1H m = one CH that is next to LOTS of hydrogens (hence the multiplet)

3H s = one CH_3 that is next to a carbon with NO hydrogens and is very close to an electron withdrawing group

2H d = this could be two identical CH's, however what would be much more probably is one CH_2 that is next to an electron withdrawing group (greater effect than with the CH_3) and is also next to a CH

With these assumptions, I've named 5 carbons and 12 hydrogens (missing a C and O) - but that carbon is the carbonyl of a ketone - and it would have no hydrogens on it, which is why it wouldn't be seen in the ^1H NMR spectrum.



Once a structure has been proposed, always check yourself by working in the other direction. In other words, what kind of spectra would you expect from this molecule.