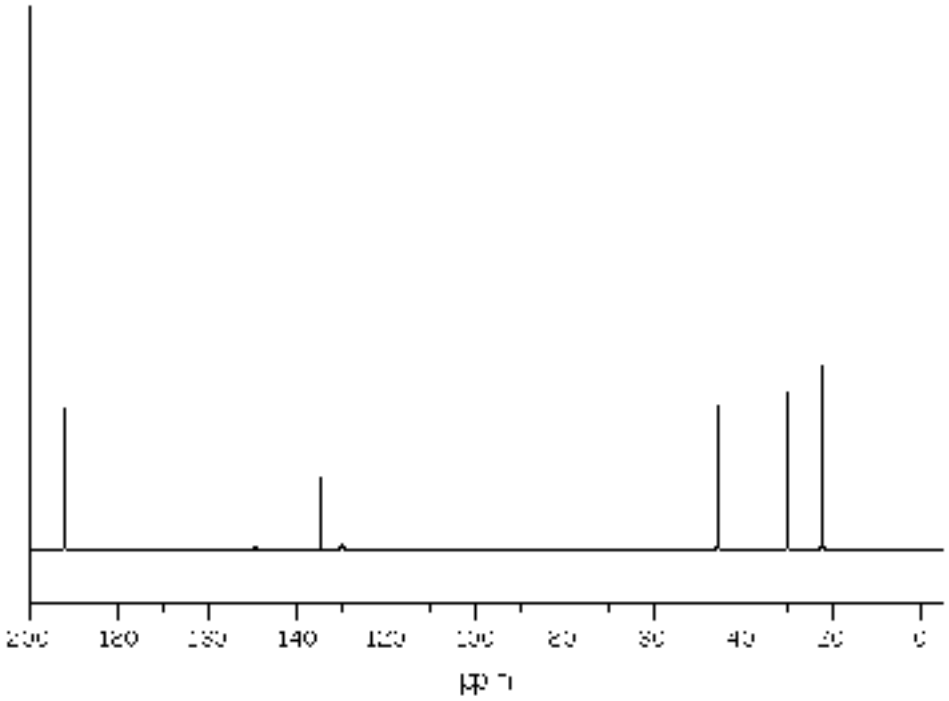
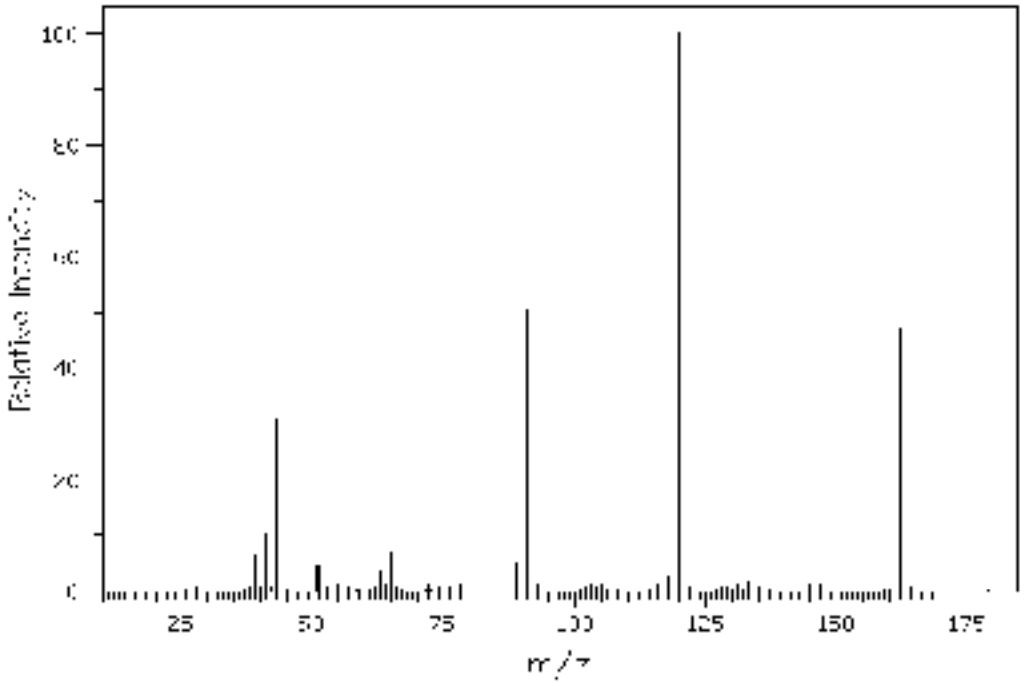
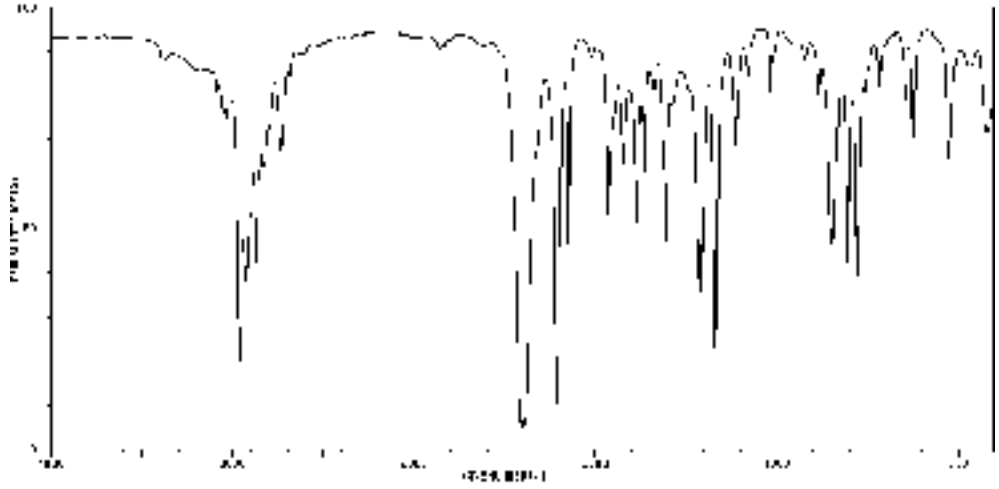


Your name: _____

What am I?





Strategy

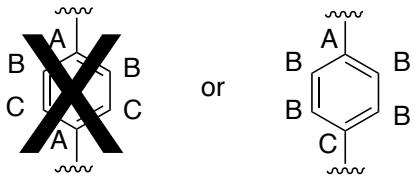
1. Try to get a molecular formula.
   a. more than likely, the molecular weight of our unknown is 162. If the mass is 163, a nitrogen must be present. Although the IR absorbance for an N-H bond shows in a similar region as does an OH, an OH absorbance is broad while an N-H absorbance is more defined (sharp). It doesn't appear as though either of these exist.
   b. other than C and H, what other atoms are in our molecule?
      i. M^+ is even, so even number of nitrogens (probably zero)
      ii. IR shows a strong C=O stretch at about 1700 cm^{-1} and maybe a small C-O near 1700 cm^{-1}. While esters and carboxylic acids have a strong C-O stretch, ketones and aldehydes only have a small C-O (because of the C-O resonance contributor). There's also no OH that would represent a carboxylic acid. Therefore there is probably only one oxygen.
      iii. Halogens not seen in mass spectrum
   c. to find molecular formula, assuming only C, H and O
      i. Subtract one oxygen from 162 (162 - 16 = 146), then and add C and H into 146.

      $C_{10}H_{26}O$ - not possible (try working through the degree of unsaturation, and prove it to yourself)
      $C_{11}H_{14}O$ - looks like a winner
      $C_{12}H_2O$ - aside from a ridiculous degree of unsaturation of 12, it's pretty hard to think of a structure with that many carbons and so few hydrogens.

2. Degree of unsaturation = 5

3. If degree of unsaturation is equal to or greater than 4, a benzene ring is likely

4. Let's confirm a benzene ring. Carbon NMR shows 3 signals in the C=C region - this must be a benzene ring that has an element of symmetry so that it has 3 electronically unique carbons. Notice that of those three peaks, one of them is HUGE and the other two are small (remember, carbon peak height is sometimes a good indicator of how many hydrogens are attached to that carbon). This probably means that the small ones that are *downfield* from the HUGE one are those that each bear a substituent. This rules out the left substitution pattern and favors that on the right (below).

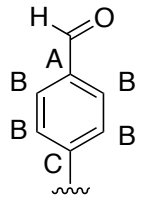


If substituents at A and C are different, then one would not typically predict all other carbon (B) signals to appear at the same chemical shift, but so be it.

There are more than one structure that can be proposed from this data.

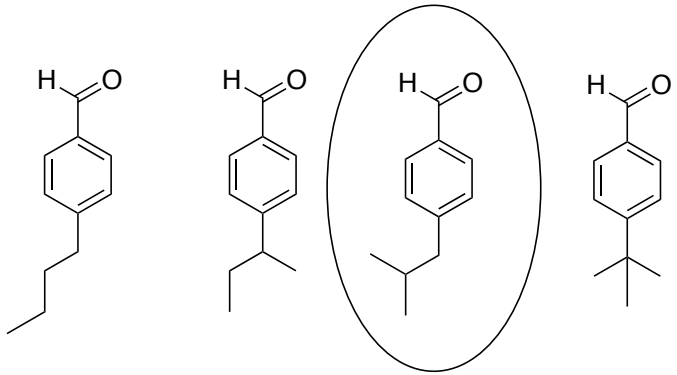
5. ^{13}C NMR confirms a carbonyl C=O a little downfield of 190. Degree of unsat. is 5; benzene ring (4) plus C=O (1) = 5. Good - all rings and/or pi bonds are accounted for.

6. The additional carbons between 50 and 20 ppm are not downfield enough to indicate they are close to the oxygen, so we should presume that the carbonyl is directly attached to the ring - this rules out a ketone, and defines the carbonyl as being an ALDEHYDE. Here's the structure, so far…

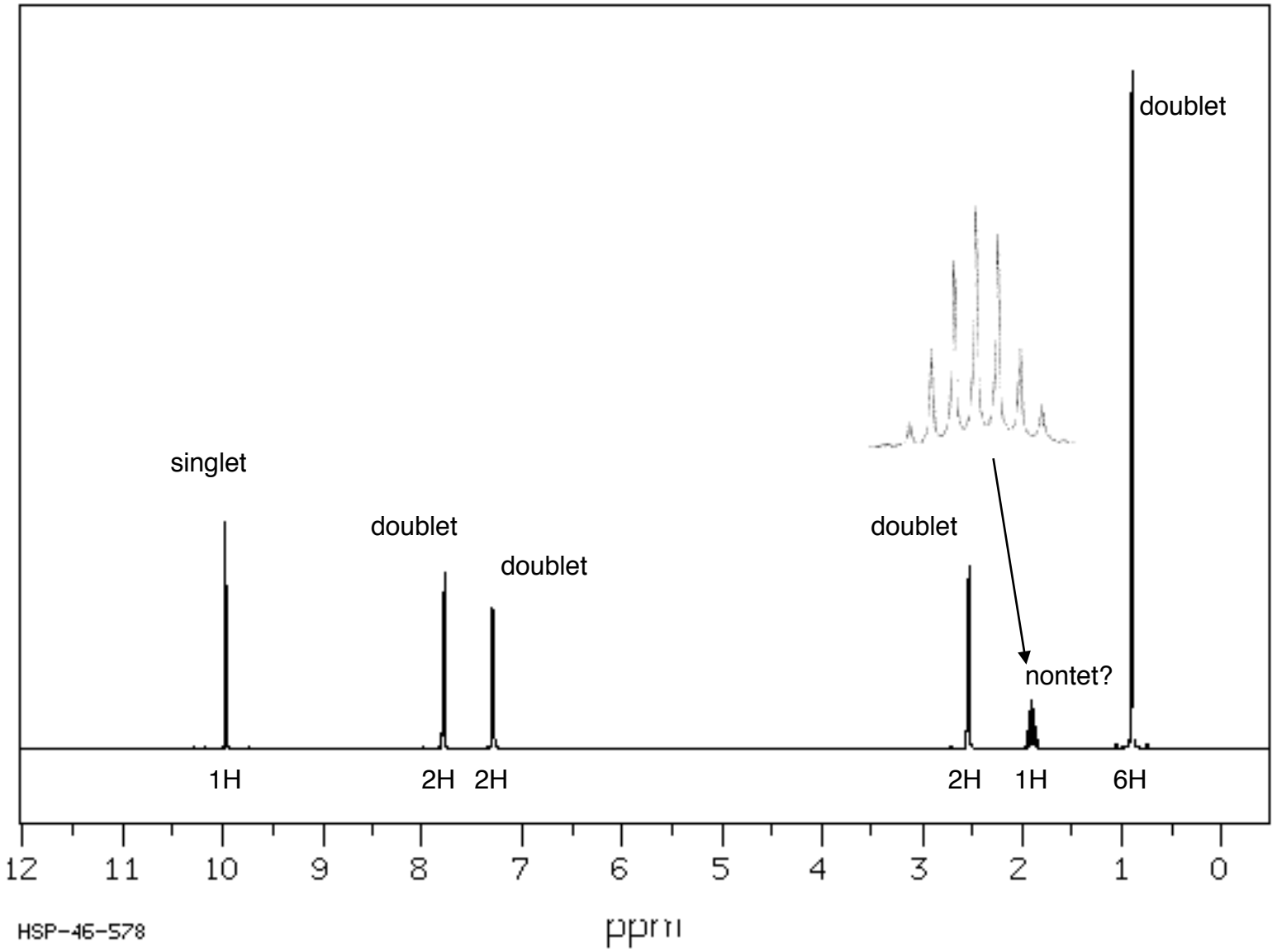


7. The structure of the 4-carbon attachment is the last thing needed.

Only the third structure matches the pattern.



That's it: 4-isobutylbenzaldehyde


doublet
singlet
doublet
doublet
doublet
nontet?
1H
2H
2H
2H
1H
6H
12
11
10
9
8
7
6
5
4
3
2
1
0
HSP-46-578
ppm