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Chapter Two, Problem A

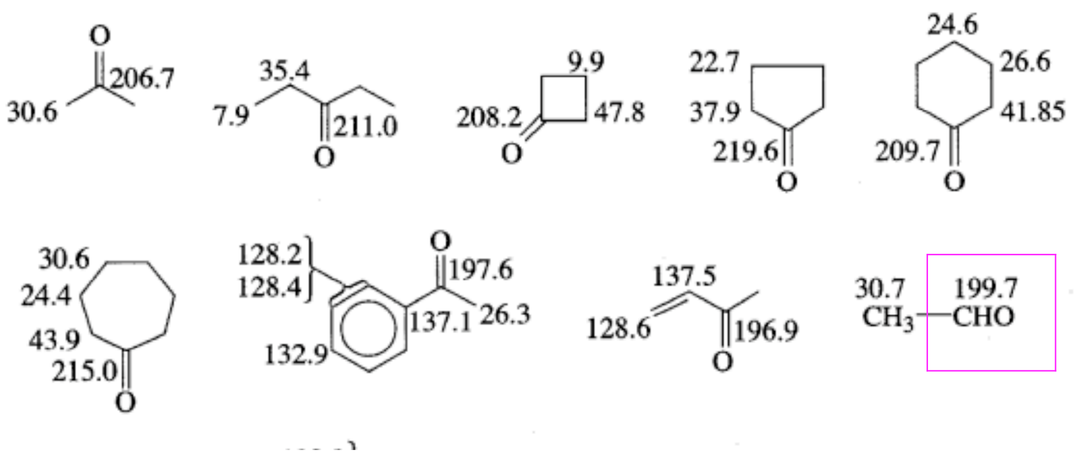
$C_7H_{12}O$

^{13}C NMR	^{1}H NMR
206.7, d	1.08, s, 6H
133.1, d	2.21, d, J = 7.2 Hz, 2H
118.4, t	5.08, d, J = 11.8 Hz, 1H
45.7, s	5.11, d, J = 15.5 Hz, 1H
41.5, t	5.75, ddt, J = 11.8, 15.5, 7.2 Hz, 1H
21.2, q (2)	9.49, s, 1H

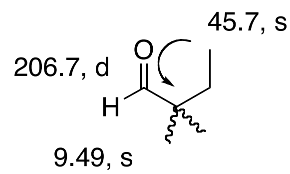
Worksheet, step one: In this case, the IHD = 2. All the H's are attached to carbon.

Worksheet, step two: We need to find out the source of the IHD. From the ^{13}C data, there is a signal at 206, which is a doublet, meaning that there is an H attached to the carbon. From the summary on the worksheet, we know that this is in the carbonyl range. Referring to Table C8, we find that this is an aldehyde.

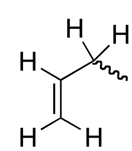
Table C.8 Shift Positions of the C=O Group and Other Carbon Atoms of Ketones and Aldehydes (ppm from TMS)



Note that the C-H of the aldehyde comes at 9.49 in the ^{1}H spectrum. It appears as a singlet, so there are no H's on the adjacent carbon. There is only one other singlet in the ^{13}C data, so that must be this carbon. That gives us an initial picture.

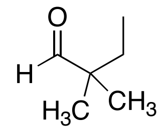


We have not yet accounted for all of the IHD. Looking further, there are two carbon signals in the alkene range, 118, t (2 H's attached), and 133, d (1 H attached). That means that we have an alkene with just one carbon attached to it. From 5.75, ddt, we know that there are two H's on the carbon adjacent to the alkene. This gives us another picture.

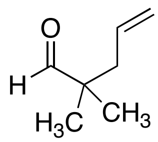


Worksheet, Step 3: There are no more heteroatoms.

Worksheet, Step 4a: There are two methyl groups, and they have the same chemical shift, so they are symmetrical. There is no other symmetry in the data, so the two methyl groups must be attached to the same carbon. They appear as a singlet in the 1H spectrum (1.08, 6H), so they are attached to a carbon with no H's. They must be attached to the carbon adjacent to the aldehyde, since there is no other singlet in the ^{13}C spectrum. So, our picture is gathering details.



Worksheet, Step 5: We have all the pieces, and there is only one way to put them together.



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