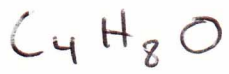


3/6/12

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→ Degree of Unsaturation

- δ 2.449, q, 2H
- δ 2.34, s, 3H
- δ 1.058, t, 3H

-Due to double bonds, triple bonds, and rings,

$$D.O.U = \frac{2C + 2 + N - X - H}{2}$$

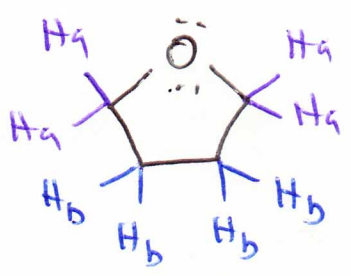
maximum # of H given # of C

2 maximum #H adjusted for heteroatoms

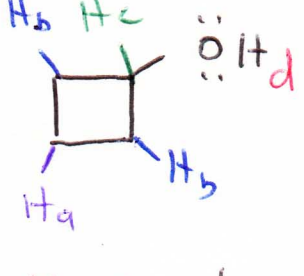
1 D.O.U

- must have a ring or C=C or C=O

what if there was a ring?



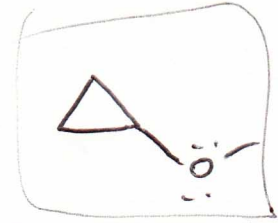
2 signals



4 signals



4 signals



3 signals, but wrong integration

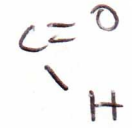


4 signals

- If there is no ring, compound must have a C=C or C=O,



δ 4.6-5.9



δ 9-10



δ 2.0-2.7

It is possible to have an alkene w/o having alkene hydrogens if the alkene is fully substituted.

Ex:



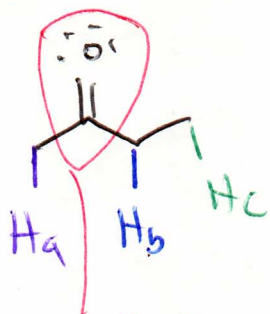
no alkene H

In this case, due to the limited # of atoms and the fact no δ > 3, there is no alkene, → must have C=O

If there is a $C=O \rightarrow$

Can only be an aldehyde if $\delta > 9$

In this case, since $\max \delta < 9$, must be a ketone.



$C=O$ blocks

Splitting

between neighbors

• $\delta 2.449, q, 2H$

• $\delta 2.34, s, 3H$

• $\delta 1.058, t, 3H$

C_4H_8O ~~$\delta 2.449$~~

heptet (7)

$\delta 9.57, d, 1H$

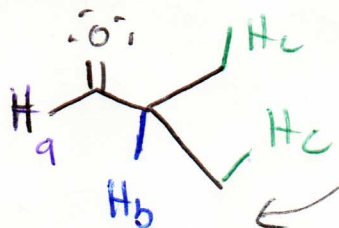
$\delta 2.39, d, hept, 1H$

$\delta 1.06, d, 6H$

The only way integration can be greater than 3 is if the molecule has some symmetry *

1 P.O.U \rightarrow ring, $C=C, C=O$

Based on $\delta \geq 9$, compound is an aldehyde, which means it has no rings or $C=C$.



Based on the splitting of the aldehyde hydrogen, there can only be exactly one H @ this position, which means the other two atoms connected must be carbons.

* Since two methyl groups are attached to the same common position, they are chemically equivalent.

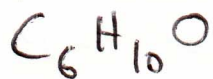
• $\delta 9.57, d, 1H$

• $\delta 2.39, d, hept, 1H$

• $\delta 1.06, d, 6H$

dt



 $\delta 2.55, t, 4H$ $\delta 2.05, tt, 4H$ $\delta 1.70, \text{quint}, 2H$

quintet (5)

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$\$D\delta$!! $\$D0$; try
try; command not found

2 D, 0, 4

- C=O + ring

- C=C + ring

- 2 rings

- C=C + C=O

- C=C + C=C

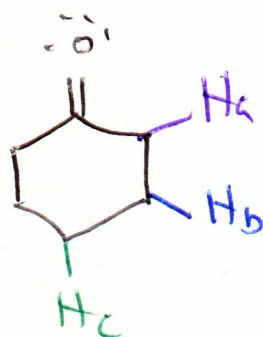
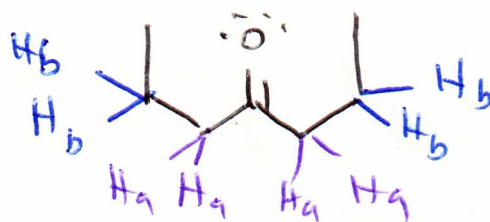
- C≡C

Compound does not have an aldehyde (no $\delta > 3$)
and, unless it is completely substituted, no alkene
(no $\delta > 3$).



Guess: ketone

Since the likely integration for the ketone H's
is 4, there must be symmetry,



- $\delta 2.55, t, 4H$
- $\delta 2.05, tt, 4H$
- $\delta 1.70, \text{quint}, 2H$