

- ⑦ Ways to ...
↳ Swelling Issues
- ⑧ T_{OH}
↳ Lack of control
- ⑨ Increased loadings
↳ Already high

HOMEWORK 4 SUPPLEMENTAL

KEY

1) MASS SPEC 216 amu (EVEN MASS)

IR] NO $>3000 cm^{-1}$ PEAK \rightarrow NO -OH OR sp, sp^2 C'S W/ H'S ATTACHED

1737 cm^{-1} PEAK \rightarrow C=O

1100 cm^{-1} PEAK \rightarrow C-O

1H nmr 3 TYPES OF H

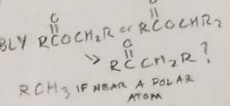
B] SINGLET: $\delta = 1.4 ppm$

SUSPECTS: $RCH_2R, R_2CH, ROH, R_2NH$

(SHIFTS AREN'T EXACT, USE MORE TO IDENTIFY WHICH H'S ARE BY POLAR ATOMS)

A] SEPTET: $\delta = 4.95 ppm$

SUSPECTS: $ROH, R_2NH, R_2C=CH_2$, POSSIBLY $RCOCH_2R$ OR $RCOCH_2R_2$



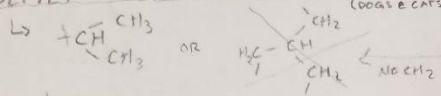
C] DOUBLET: $\delta = 1.15 ppm$

SUSPECTS: ROH, R_2NH, RCH_2R , POSSIBLY RCH_3

SEPTET * DOUBLET MUST SPLIT EACH OTHER (DOGS & CATS)

INTEGRAL: A:B:C \approx 1:3:6

(JUST AIM FOR WHOLE #'S)



^{13}C nmr 5 TYPES OF C

2 PEAKS VANISH \Rightarrow 2 QUARternary C'S (δ INDICATES $RCOR$ OR R^2C)

\rightarrow ONE IS VERY DOWNFIELD

3 PEAKS STAY SAME \Rightarrow 3 C'S W/ 3 OR 1 H

THOSE ARE THE "STRUCTURAL ELEMENTS" (CLUES) ABOVE, NOW ANALYZE & GUESS

IF NO N (NO OBVIOUS CLUES N IS PRESENT LIKE ODD MASS OR COMBUSTION ANALYSIS)

IF [A] & [C] H'S ARE $\begin{matrix} CH_3 \\ | \\ CH \\ | \\ CH_3 \end{matrix}$, INTEGRATION RATIOS INDICATE [B] IS $\begin{matrix} CH_3 \\ | \\ CH \\ | \\ CH_3 \end{matrix}$

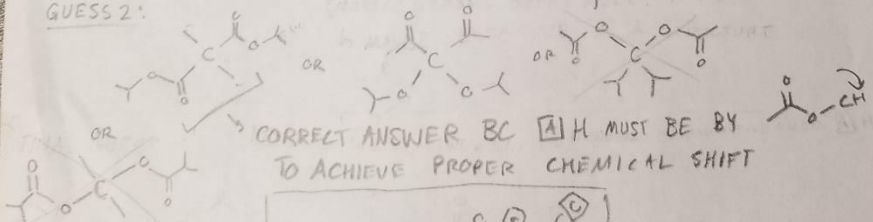
\rightarrow NO C'S W/ H'S LEFT BY 1H nmr, SO ONLY C'S LEFT ARE QUARternary

\rightarrow IF C=O EXISTS, IT MUST NOT HAVE AN H ATTACHED $\rightarrow R^2C=O$ OR $R^2C=O$ OR RO^2C

GUESS 1: $\begin{matrix} O \\ || \\ C \\ | \\ O \end{matrix}$ [NO B/C MASS = 102, IF STRUCTURE IS DOUBLED, MASS = 204, \neq 216-204 = 12] \rightarrow C?!

\rightarrow CONNECT "DOUBLED STRUCTURE W/ MISSING QUARternary C" \rightarrow PICK A PLACE TO "BREAK" & INSERT QUARternary C

GUESS 2:



\rightarrow SEPTETS δ NOT DOWNFIELD ENOUGH

