Chem 744

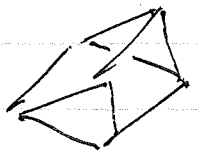
Homework #1 - Key

(1) 
A

Symmetric - all C's equivalent.
UV-Vis shows peaks due to conjugated π-system.


B

2 different Carbons.
No π-conjugation.


C

All C's equivalent
No π bonds ≡ No UV-Vis

(2) C $\frac{88.2\text{ g}}{12.011\text{ g/mol}} = 7.34$ $\frac{7.34}{7.34} = 1$

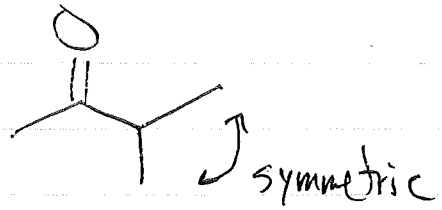
H $\frac{11.7\text{ g}}{1.008\text{ g/mol}} = 11.6$ $\frac{11.6}{7.34} = 1.5$

$\Rightarrow$ empirical Formula $\boxed{C_2H_3}$

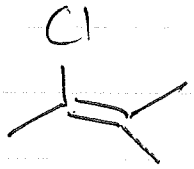
C_2H_3 MW = 27

Mass $\frac{136}{27} = 5 \Rightarrow C_{2\times5}H_{3\times5}$

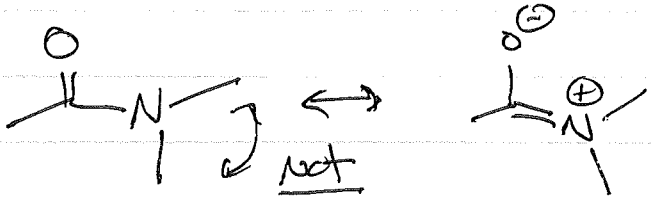
$\Rightarrow$ $\boxed{C_{10}H_{15}}$

(3) 

2-CH_3's



All CH_3's different cis/trans



equivalent

Slow amide Rotation

(4) a) $\frac{414\ Hz}{300\ MHz} = 1.38\ ppm$

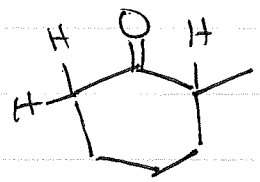
$\frac{660\ Hz}{25\ MHz} = 26.4\ ppm$

(5) O_2 is a triplet in the ground state $\cdot\ddot{O}-\ddot{O}\cdot$
Unpaired electrons affect T_2 Relaxation
increasing T_2 rate leads to broadening.

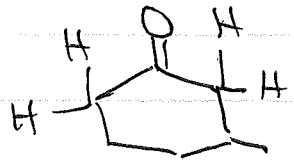
(6) ONLY C $\frac{720}{12} = 60$ 1 peak - symmetric

C_{60} - Buckminsterfullerene

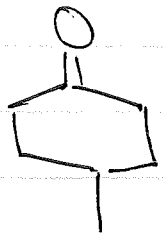
(7) a) N-H would show and additional H on Proton NMR

b) 

3 H's downfield
Not symmetric

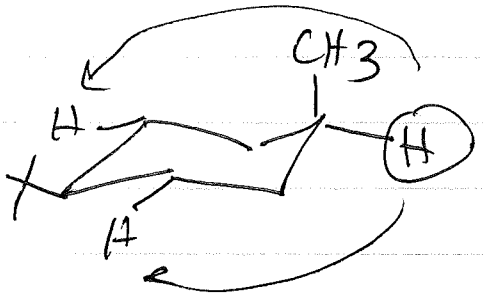


4 H's downfield
Not symmetric



Symmetry
^1H + ^{13}C

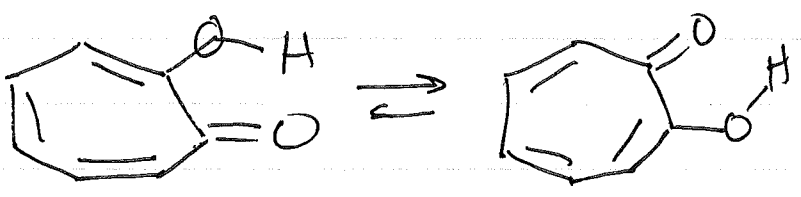
c) trans coupling J will be larger for the H-H. Cis will be smaller.

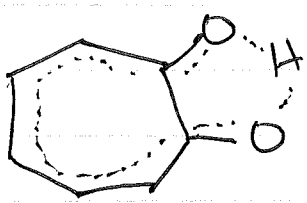
d) 

equatorial H will have additional W-coupling

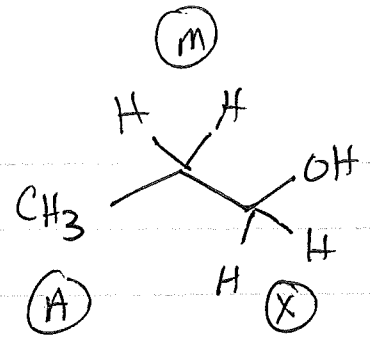
e) In ^{13}C the Br heavy atom effect will shift C upfield.

(8) We are seeing the average spectra. symmetric.



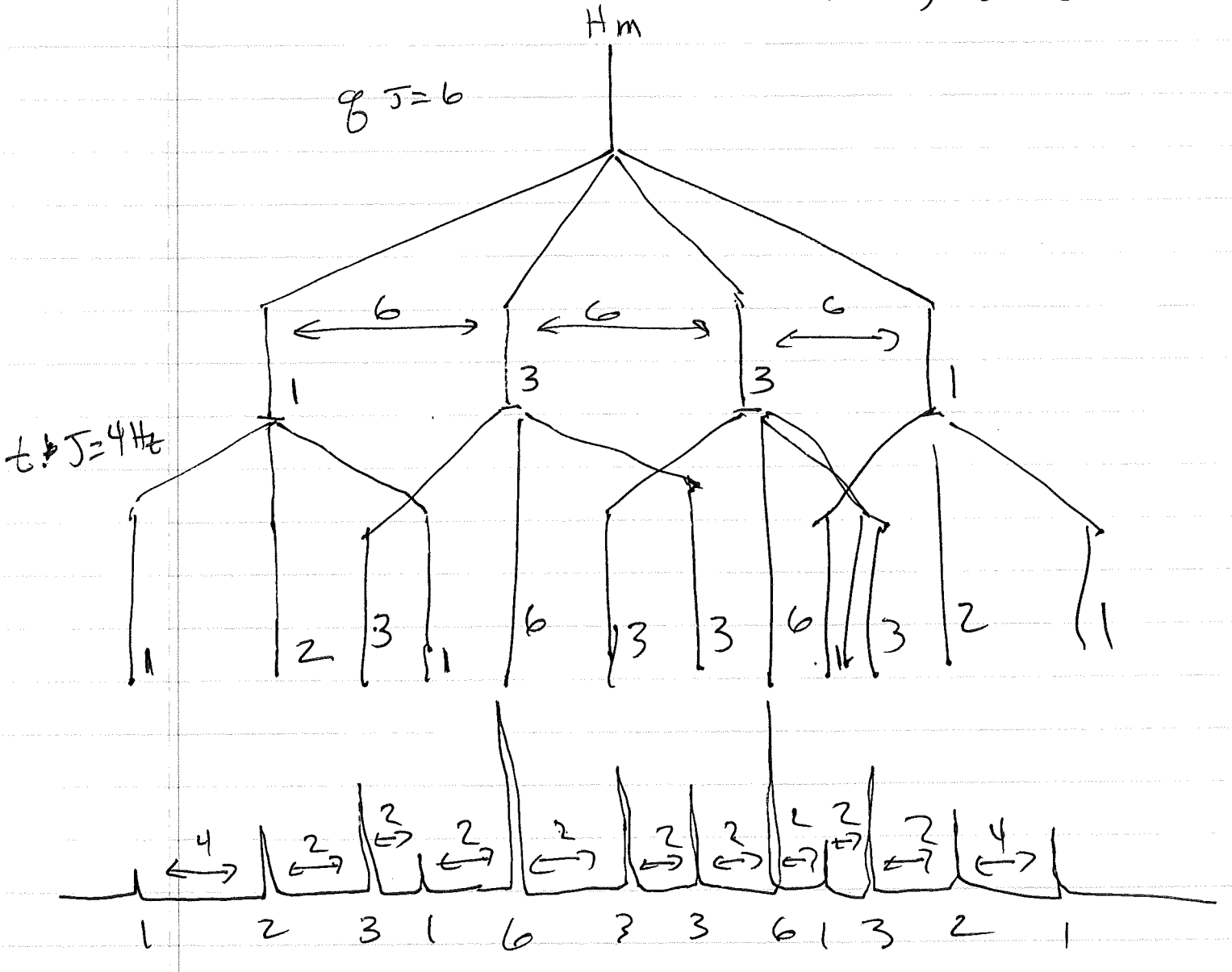


(9)



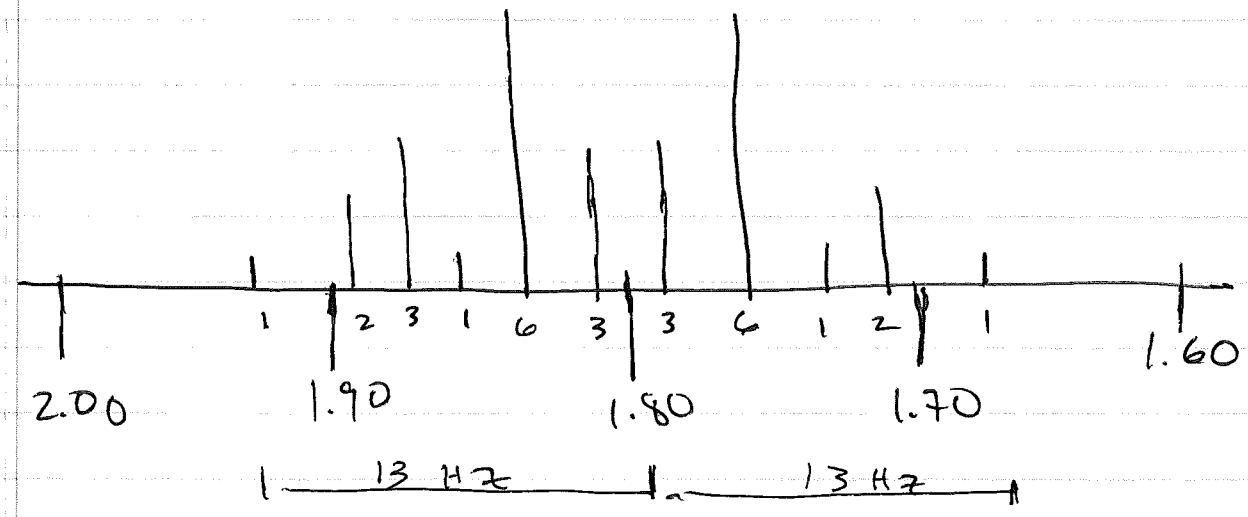
$A_3M_2X_2$

$H_M \equiv$ triplet of quartets.
$J = 4\,Hz, 6\,Hz.$

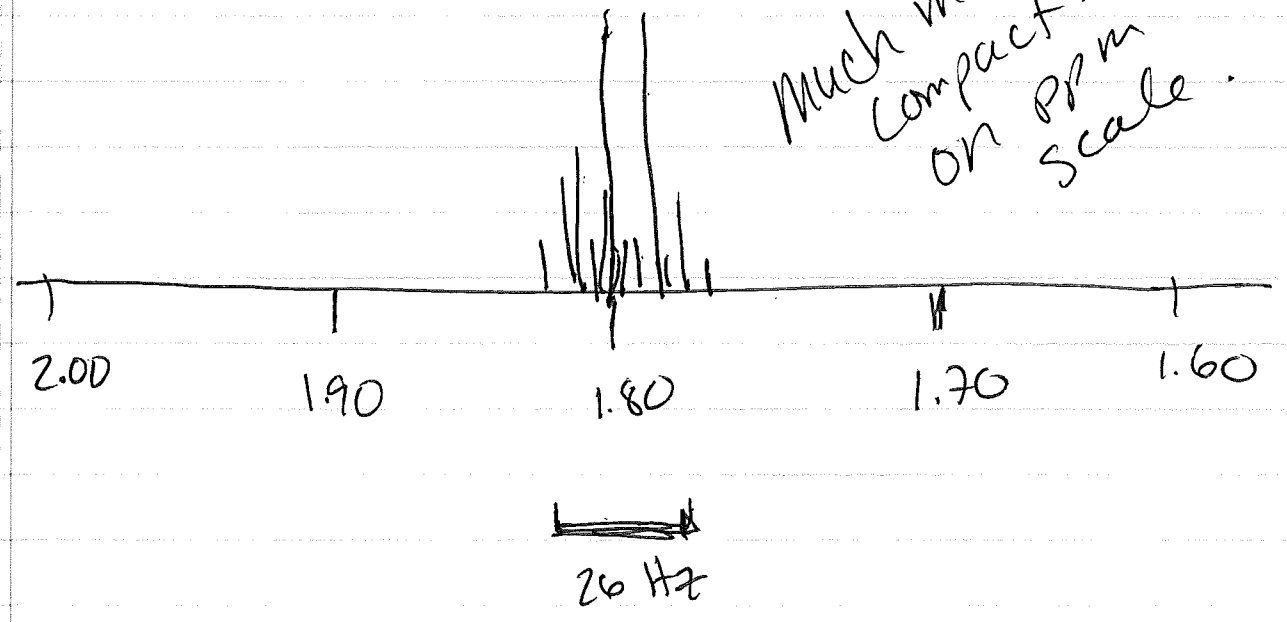


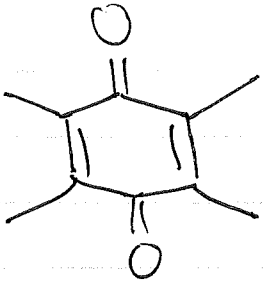
total 26 Hz

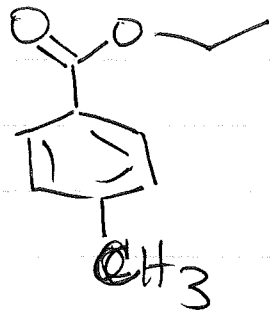
100 MHz (100 Hz per ppm)
(10 Hz per 0.1 ppm)

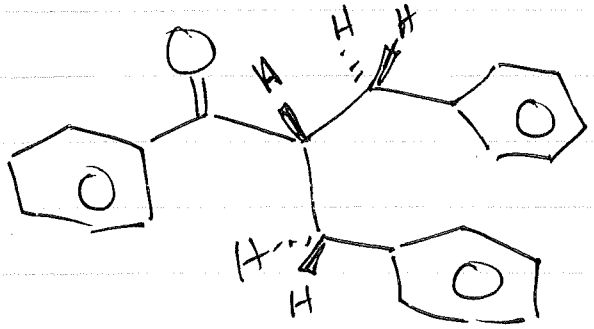


500 MHz (500 Hz per ppm
50 Hz per 0.1 ppm)



(10) a) 

b) 

(11) 

Note: Unusual Coupling of CH_2's.

A rare case of diastereotopic protons in a symmetric molecule without a stereogenic center.