HOMEWORK - 1 KEY

CHEM 744
SPRING 2019

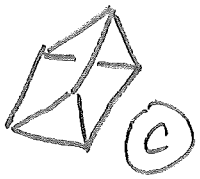
(1)

(A)

All carbons equivalent - sp^2
UV-vis shows π-conjugation.

(B)

2 different types of carbon.
no π-conjugation.



(C)

symmetric - 1 carbon - sp^3
No π-conjugation.

(2)

Assume 100g sample.

C $\dfrac{88.2\ g}{12.011\ g/mol} = 7.34$ $\qquad \dfrac{7.34}{7.34} = 1$

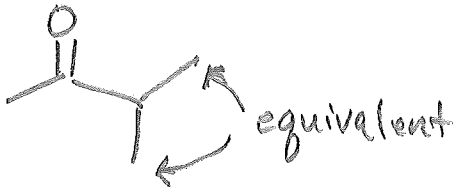
H $\dfrac{11.7\ g}{1.008\ g/mol} = 11.6$ $\qquad \dfrac{11.6}{7.34} = 1.5$

$\Rightarrow$ emperical formula $\boxed{C_2H_3} \Rightarrow$ mass = 27

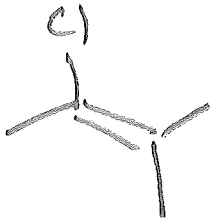
mass $\dfrac{136}{27} = 5 \Rightarrow C_{2\times5}H_{3\times5}$

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

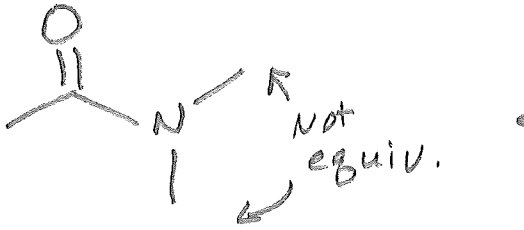
(3)

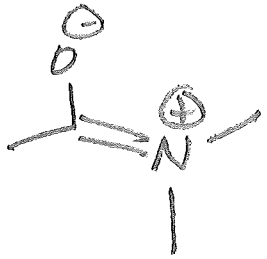


2 different CH_3's



All CH_3's different





3 diff. CH_3's

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

b) $\frac{600\ Hz}{25\ MHz} = 26.4\ ppm$

(5) O_2 is a triplet in the ground state. 

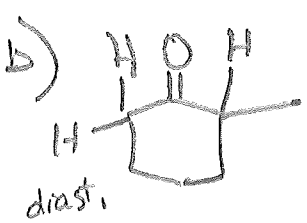
Unpaired electrons affect T_2 Relaxation Leading to broadening.

(6) only C $\frac{720}{12} = 60$ 1 peak ⇒ Symmetric

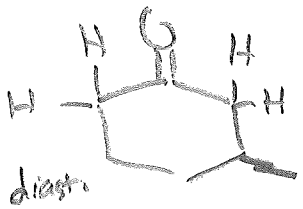
C_{60} - Buckminster Fullerene

(7) a) N-H would appear on proton NMR.

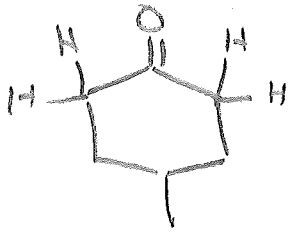
b)



3 H's downfield
Not symmetric
7-carbons



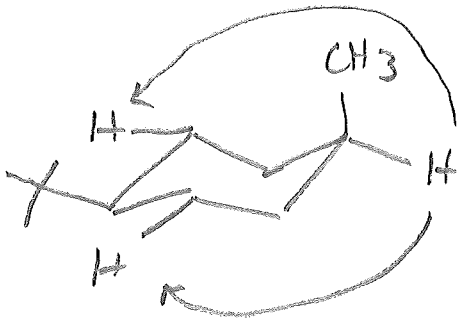
4 H's downfield
Not Symmetric
7-carbons



Symmetric
5-carbons

c) trans coupling will be larger J.

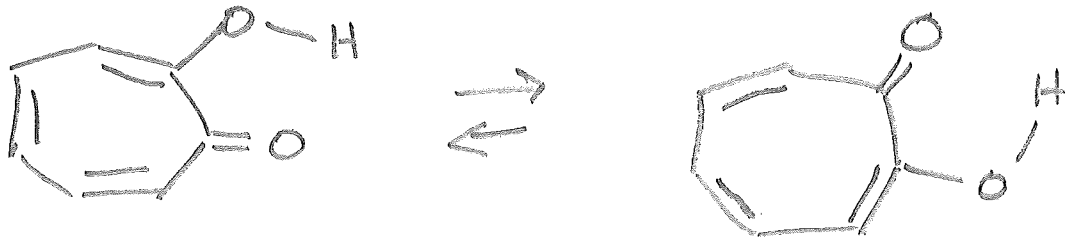
d)



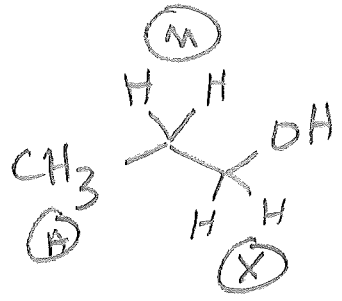
equatorial H will have long range w-coupling.

e) In ^{13}C-NMR the bromo-compound will have an upfield shift due to Heavy atom effect shielding.

(8) We are seeing an average spectra of rapidly equilibrating tautomers.



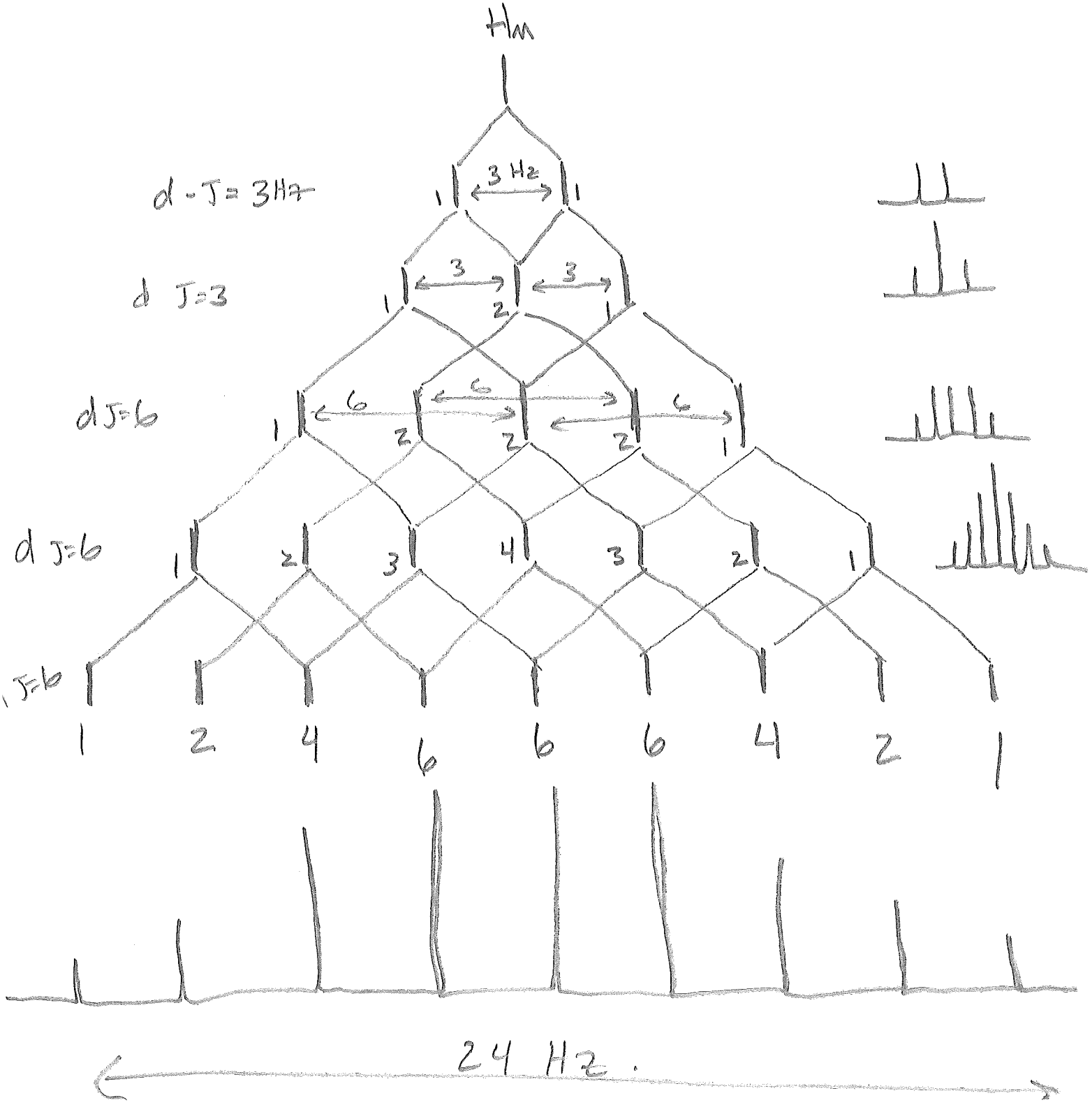
(9)



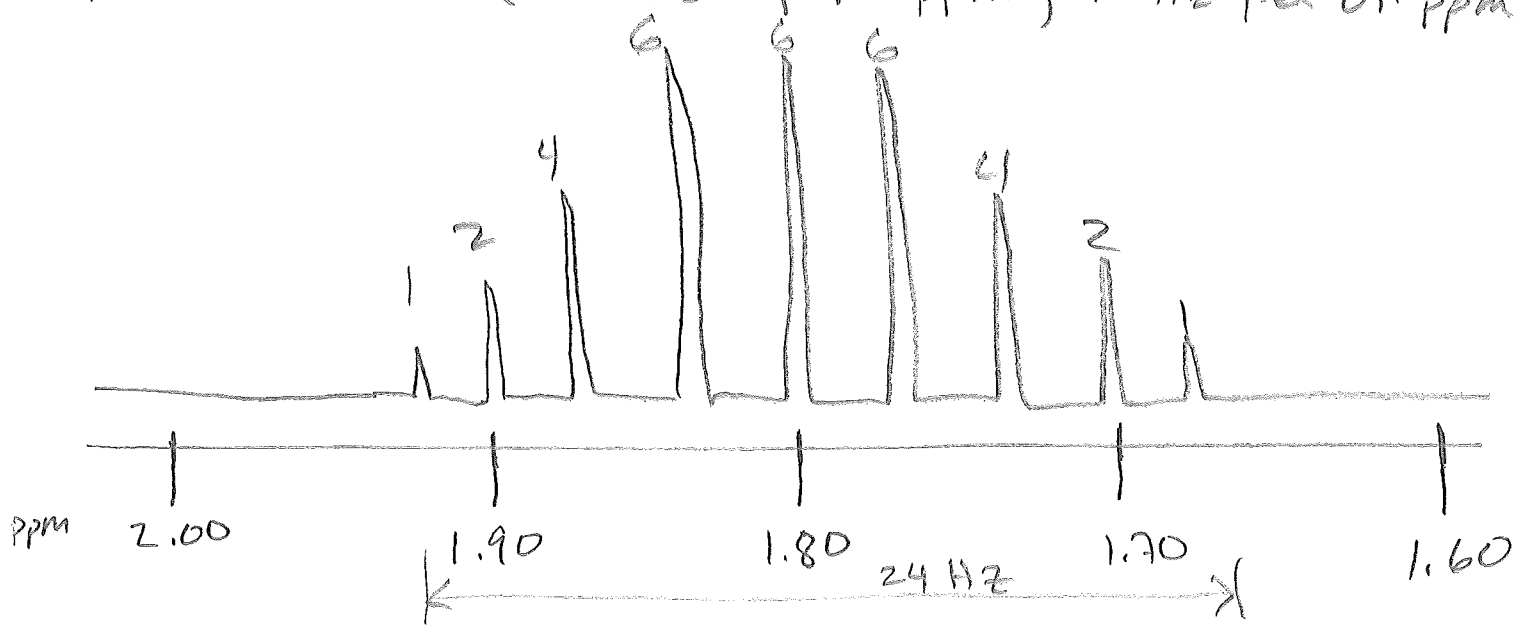
$A_3M_2X_2$

dd ddd

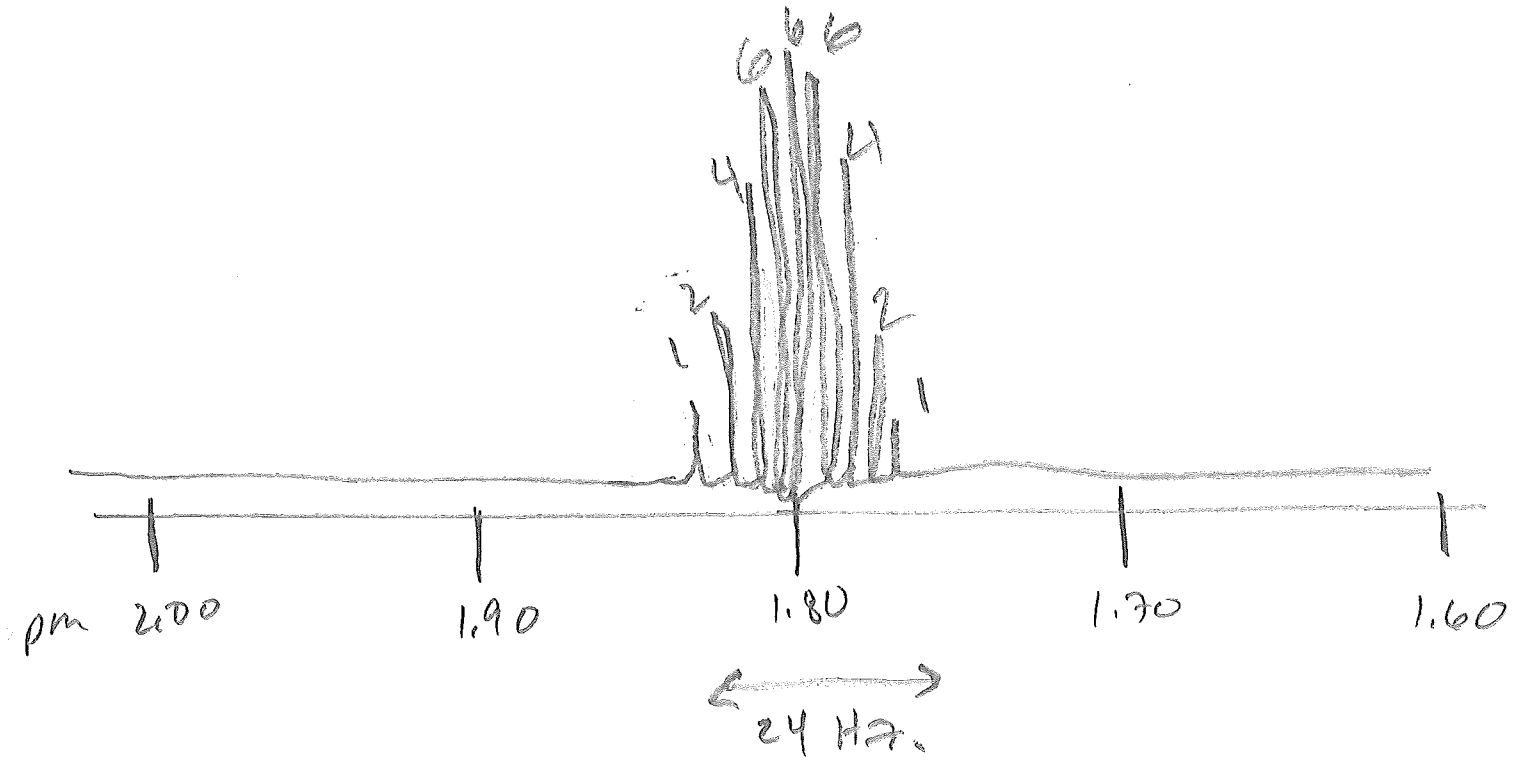
H_M = tq J = 3, 6 Hz



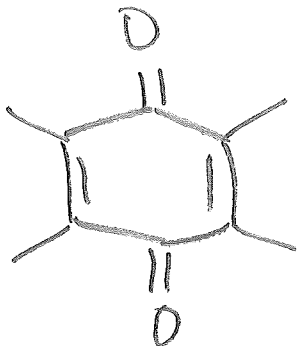
100 MHz (100 Hz per ppm, 10 Hz per 0.1 ppm)



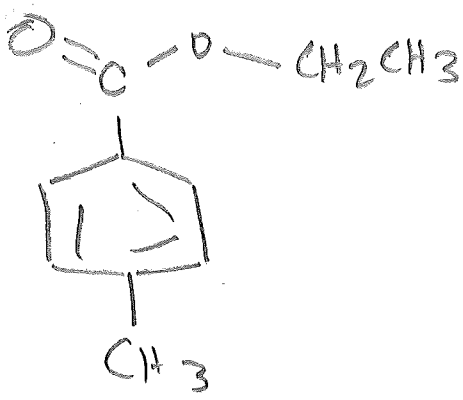
500 MHz (500 Hz per ppm, 50 Hz per 0.1 ppm)



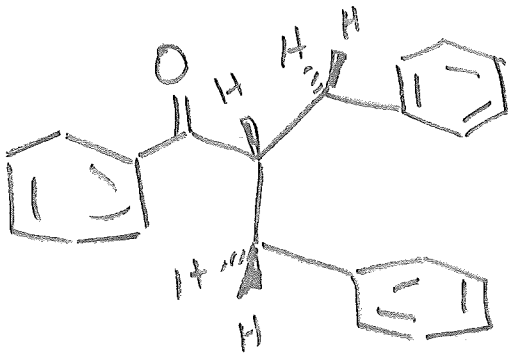
(10) a)



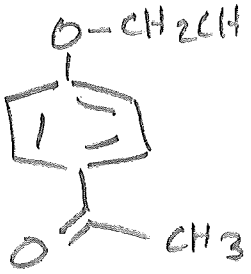
b)



(11)



Note: would be hard to distinguish from this Ketone without more information.



lack of symmetry in NMR is deceiving. the CH_2's have diastereotopic H's even though the molecule does not have a center of chirality.

Unusual case of non-equivalent protons due to magnetic non-equivalence.