Chem 333

Name____Key_____

Fall 2012
Exam #2
October 22, 2012

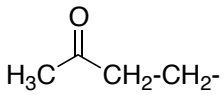
1. (20 points) $C_8H_{15}BrO$

^{13}C NMR:	**^{1}H NMR:**
208.2, s	4.13, tq, J=1.5, 6.3 Hz, 1H
51.2, d	2.45, t, J=7.3 Hz, 2H
43.2, t	2.14, s, 3H
40.7, t	1.70, d, J=6.3 Hz, 3H
29.8, q	1.3-1.8, m, 6H
27.1, t	
26.3,q	
22.9, t	

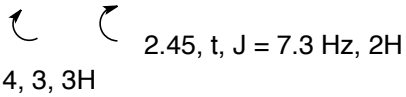
1. IHD = 1
   All H's attached to carbon

2. Ketone at 208.2, s

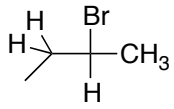
From generic chemical shifts, have



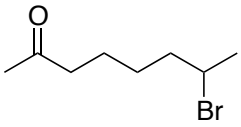
This is confirmed in the ^{1}H NMR. We also see there is an additional CH_2



3. We have an additional Br. From generic chemical shifts, this must be the 51.2, d. This is confirmed in the ^{1}H NMR, 4.13, tq, J = 1.5, 6.3 Hz, 1H. So, the methyl group must also be attached, and there must be an additional CH_2.



5. Putting it all together



2. (40 points)

$C_6H_{13}NO_2$

^{13}C NMR:

109.1, s
77.4, d
66.9, t
44.7, t
26.8, q
25.3, q

^{1}H NMR:

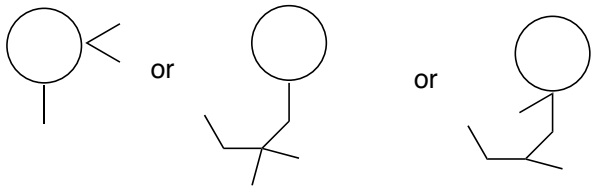
4.13, m, 1H
4.00, dd, J=6.6, 8.1 Hz, 1H
3.67, dd, J=6.3, 8.1 Hz, 1H
2.85, dd, J=4.2, 13.2 Hz, 1H
2.78, dd, J=6.0, 13.2 Hz, 1H
1.40, s, 3H
1.34, s, 3H
1.31, bs, 2H (exchanges)

1. IHD = 1

Two H's not attached to C: OH + NH, OH + OH, or NH_2

These appear together at 1.31, bs, 2H (exchanges)

2. No carbonyls or alkenes, so must be ring



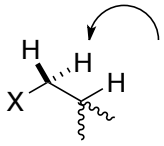
3. From ^{13}C, two oxygenated carbons, and one aminated

$O-CH_2$	O−CH	$N-CH_2$
66.9, t	77.4, d	44.7, t

also have 109.1, s = carbon with two heteroatoms attached

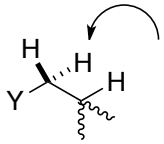
4. a. Two methyl groups, both attached to the C with no H's, but not symmetrical

b. We have two independent spin systems



2.85, dd, J=4.2, 13.2 Hz, 1H
2.78, dd, J=6.0, 13.2 Hz, 1H

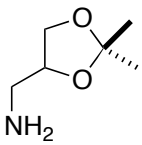
From chemical shift, X = N



4.00, dd, J=6.6, 8.1 Hz, 1H
3.67, dd, J=6.3, 8.1 Hz, 1H

From chemical shift, Y = O

5. Putting it all together



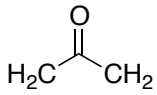
3. (40 points) $C_9H_{14}O$ **IR:** 1715, 1640, 915 cm^{-1}

^{13}C NMR:	**^{1}H NMR:**
211.2, s	1.2-2.3, m, 11H
135.4, d	4.99, d, J = 10.9 Hz, 1H
116.5, t	5.02, d, J = 15.5 Hz, 1H
47.4, t	5.61, ddt, J = 10.9, 15.5, 7.6 Hz, 1H
41.1, t	
40.5, d	
38.5, t	
30.6, t	
24.9, t	

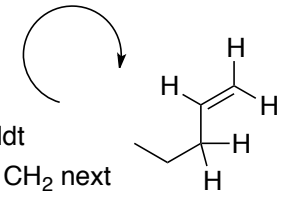
1. IHD = 3

all H's attached to carbon

2. From 211.2, s have ketone. From generic chemical shifts, have



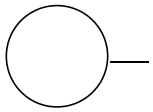
From 116.5, t and 135.4 d have



5.61, ddt

tells us CH_2 next to alkene

Must also have a ring, with a single branch:



The end group on the branch is the alkene. The carbonyl must be part of the ring, as there is no symmetry From 1715 cm^{-1}, ring must be at least six-membered.

5. Putting it all together: