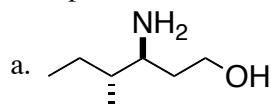
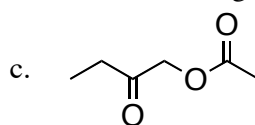


Fall 2008
Homework #3
KEY

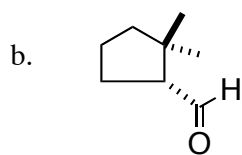
1. (12 points) Write out IUPAC names for each of the following:



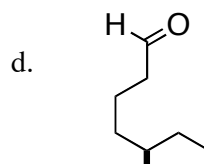
(3S, 4R)-3-amino-4-methyl-1-hexanol



2-oxobutyl propanoate

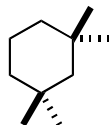
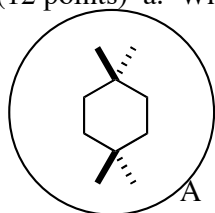


(1R)-2,2-dimethylcyclopentanecarbaldehyde

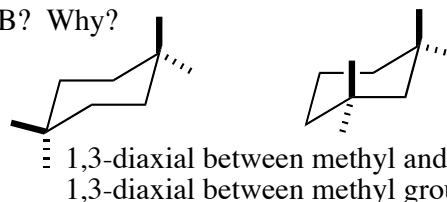


(5R)-5-methylheptanal

2. (12 points) a. Which is more stable, A or B? Why?

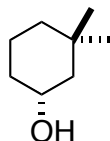
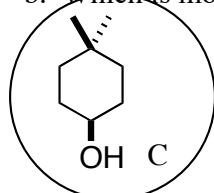


B

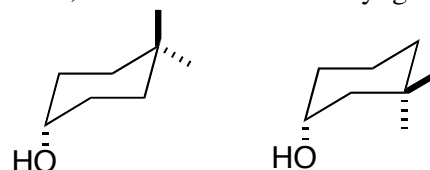


1,3-diaxial between methyl and H (A) is less costly than 1,3-diaxial between methyl groups (B)

b. Which is more stable, C or D? Why?

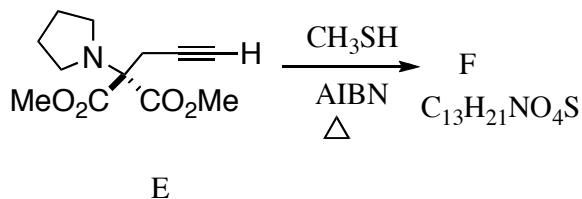


D



The more stable chairs are the same. For the less stable chairs, 1,3-diaxial between OH and H (C) is less costly than 1,3-diaxial between OH and methyl (D)

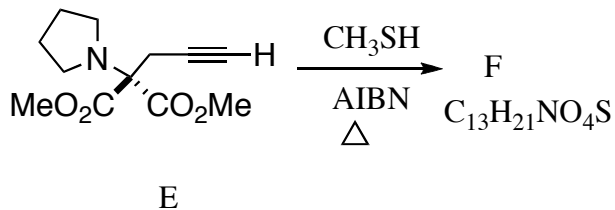
3. (6 points) Reaction of **E** with CH_3SH gives **F**. Deduce the structure of **F**, and draw an arrow-pushing mechanism for the transformation of **E** to **F** (on back). Hint: the first step is H atom removal from the CH_3SH .



E

^{13}C NMR

171.8, s	44.0, d
171.4, s	43.0, t
75.4, s	37.4, t
71.9, d	31.9, t
52.6, q	28.6, t
52.3, q	18.5, q
48.6, t	



¹³C NMR

171.8, s	44.0, d
171.4, s	43.0, t
75.4, s	37.4, t
71.9, d	31.9, t
52.6, q	28.6, t
52.3, q	18.5, q
48.6, t	

Analysis: From the formula, CH₃SH has been added. The alkyne is gone, and so is the symmetry (ring, esters) of the starting material, suggesting that the ring has been substituted, and that the carbon where the esters are attached is also a part of a ring.

Presumably the C-N ring is still there. The CH₂'s of that ring before cyclization would have been at 47, t (2) and 27, t (2). The 48.6, t in the product is likely the ring CH₂ next to the N. If the other carbon next to the N were substituted, it would be a doublet further downfield, 71.9, d. The 75.4, s is the carbon to which the two esters is attached.

The CH₃S is at 18.5, q. The other carbon of the sulfide could be at 34, t; 46, d; or 52, s. This leads to two plausible structures, **E** and **F**. **E** was the right answer, but full credit was given for **F**.

