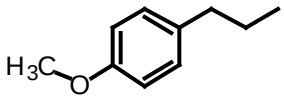
CHE 173
Winter, 2005
Quiz 2 Answer Key

Name_____

Section: 201 202 203 204 205
M T W Th F
(circle one)

1. For the compound shown below, draw the:



(a) ^{1}H NMR spectrum (10 points)

triplet at 1.0 ppm (3H) for the side-chain methyl protons
sextet at 1.2 ppm (2H) for the side-chain methylene protons
triplet at 2.2 ppm (2H) for the benzylic methylene protons
singlet at 3.5 ppm (3H) for the methoxy protons
doublet at 7.0 ppm (2H) for one set of aromatic ring protons
doublet at 7.4 ppm (2H) for the other set of aromatic ring protons

(b) ^{13}C NMR spectrum (10 points)

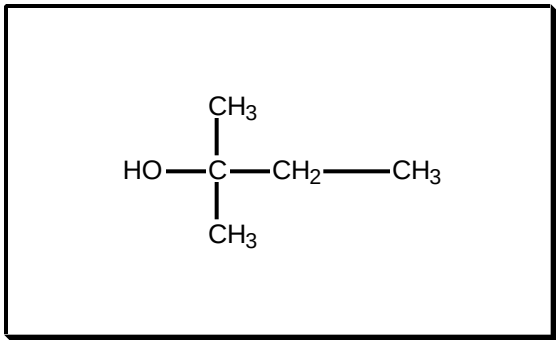
There should be 8 signals in all, all singlets with the following chemical shifts: δ 10 (for the side-chain methyl), 15 for the side-chain methylene, 35 (for the benzylic methylene), for sets of aromatic carbons in the range of 110-145, and 80 (for the methoxy group).

(c) off-resonance decoupled ^{13}C NMR spectrum (10 points)

The off-resonance decoupled 13C spectrum shows the splitting of the carbon signal that results from attached protons. So, there should be a quartet at 10, triplet at 15, triplet at 35, two doublets and two singlets in the aromatic region, and a quartet at 80 ppm.

2. A compound gives the IR, MS, ^{1}H and ^{13}C NMR data shown on the next page.

(a) Identify the structure of the compound (10 points)



(b) Explain your structure making reference to key features from each of the spectra provided (10 points)

The molecular formula is given. The molecular ion is at 88 with a significant peak at 73 (M-15, or a methyl group) and the base peak is at 59 (M-29, or an ethyl group). The IHD = 0, so the compound is saturated (no rings or double bonds). The broad absorption band at 3376 cm^{-1} in the IR suggests an OH group; CH stretching is observed for sp^3 - hybridized carbons only. The carbon NMR shows 4 unique carbons present (DEPT confirms two CH_3, one CH_2 and a C). The proton NMR shows 4 unique types of protons, including a classic triplet-quartet splitting pattern for an ethyl group. The singlet in the proton NMR spectrum at 1.2 ppm integrates for 6 protons (2 methyl groups). Putting it all together, the structure shown above is consistent with all the data.