CHM 3150L Organic Laboratory, Dr. Laurie S. Starkey NMR Problem Set #1: Predicting IR and ¹H NMR Spectra

Name:_____

For each of the following molecules, predict what you would find in its IR spectrum and its 1 H NMR spectrum. For the IR, <u>list the significant peaks</u> which are expected, and indicate which functional group is responsible for that peak (e.g., O-H stretch around 3300 cm⁻¹). For the 1 H NMR, each unique type of proton has already been indicated (a, b, etc.). For each signal, determine how many H's (peak integration) and what the splitting pattern would be, and then <u>estimate</u> and/or <u>calculate</u> the expected chemical shift (δ value in ppm, **show your work**).

proton #H, split δ (ppm)

5H, singlet \sim 7ppm (aromatic)

b 2H, triplet ~ 2.3 ppm (benzylic) or calculate $\delta = 1.2 + 1.4$ (Ar) + 0.0 (R) = 2.6 ppm

IR peaks:

d

c

e

CH₃O CH₃II CH₃-C-C-O CH₂ CH₃

IR peaks:

proton #H, split δ (ppm)

a

b

c

d

 $\begin{array}{c|c}
& b & c & 0 \\
& a & b & c & 0 \\
& c & d & c \\
& C & || \\
& C &$

proton #H, split δ (ppm)

a

b

c

d

e

f