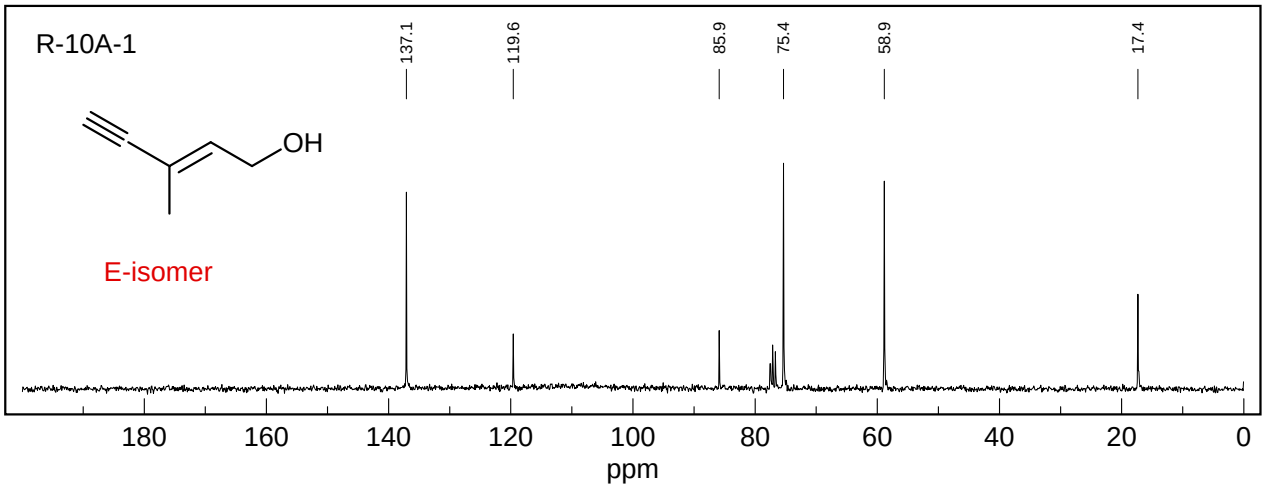
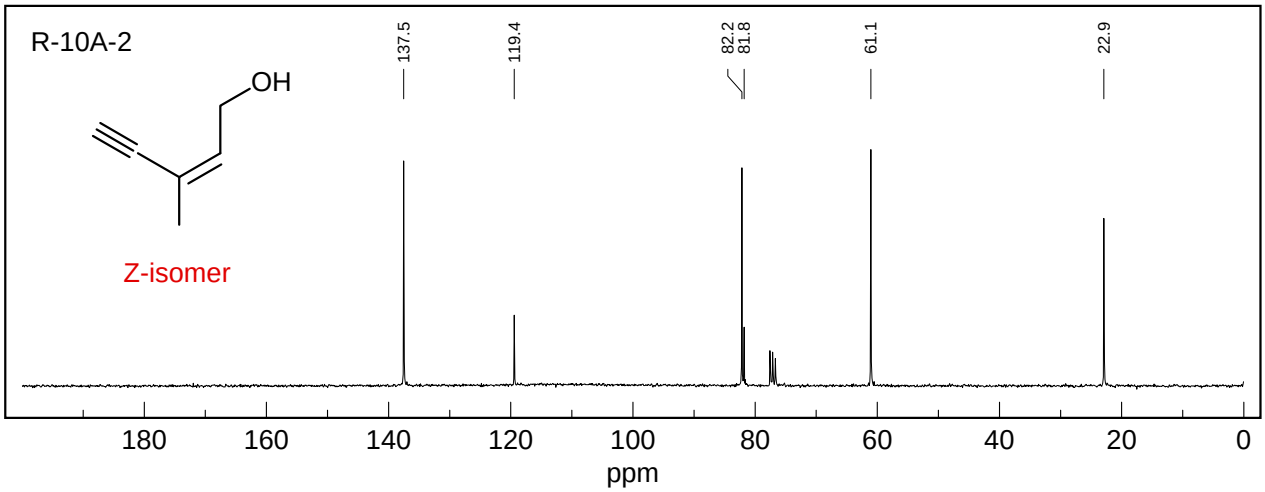
Problem R-10A (C_6H_8O)

75 MHz ^{13}C NMR spectrum in $CDCl_3$

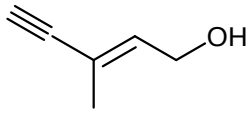
Source: Aldrich Spectra Collection/Reich g



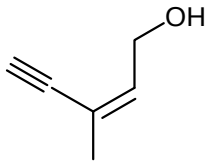


7

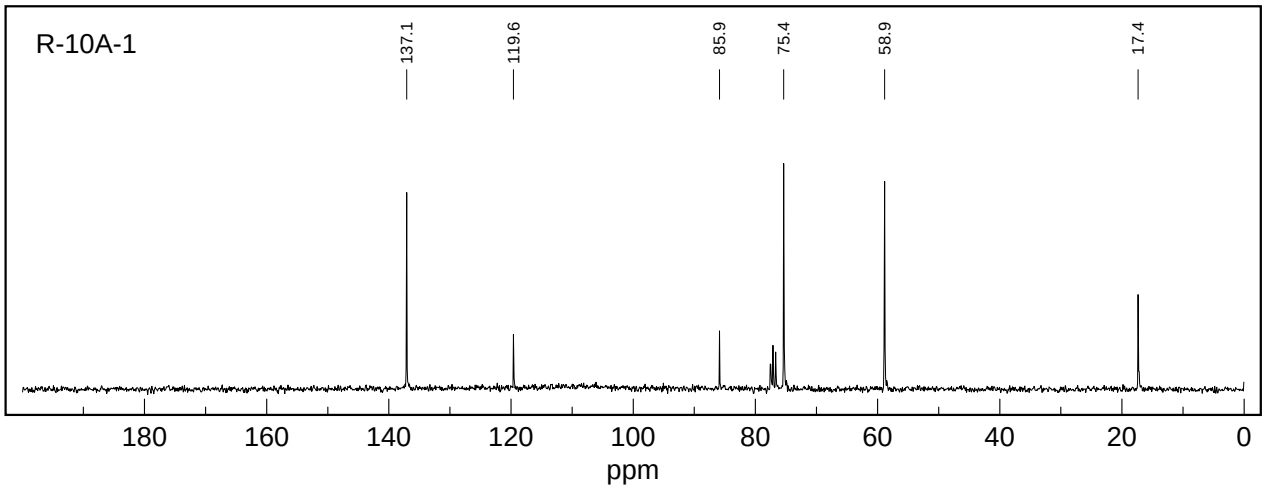
Problem R-10A (C_6H_8O). Below are given the ^{13}C NMR spectra of two stereoisomers of 3-methyl-pent-2-ene-4-yn-1-ol. Assign structures, and assign the signals by writing the δ values next to the appropriate carbons on each structure (Source: Aldrich Spectra Viewer).

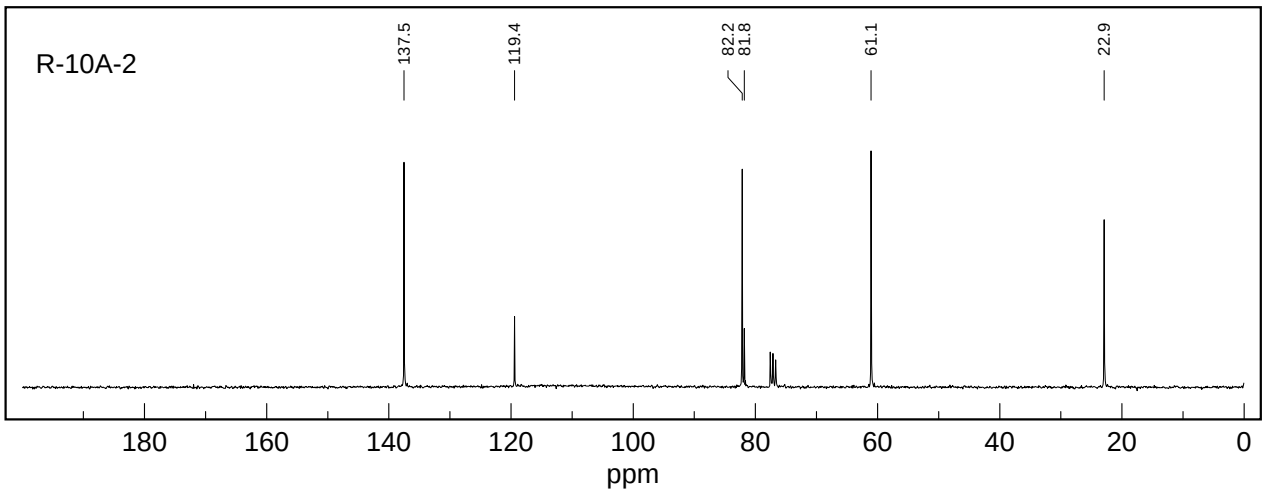


R-10A-__



R-10A-__

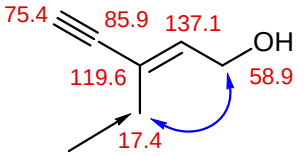




Briefly explain the basis for your assignment. Be specific.

7

Problem R-10A (C_6H_8O). Below are given the ^{13}C NMR spectra of two stereoisomers of 3-methyl-pent-2-ene-4-yn-1-ol. Assign structures, and assign the signals by writing the δ values next to the appropriate carbons on each structure (Source: Aldrich Spectra Viewer).

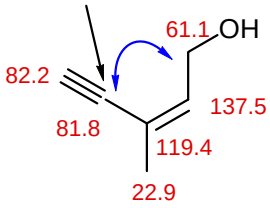


γ-effect, CH_3 should be upfield (-5.5 ppm)

E-isomer

R-10A-**1**

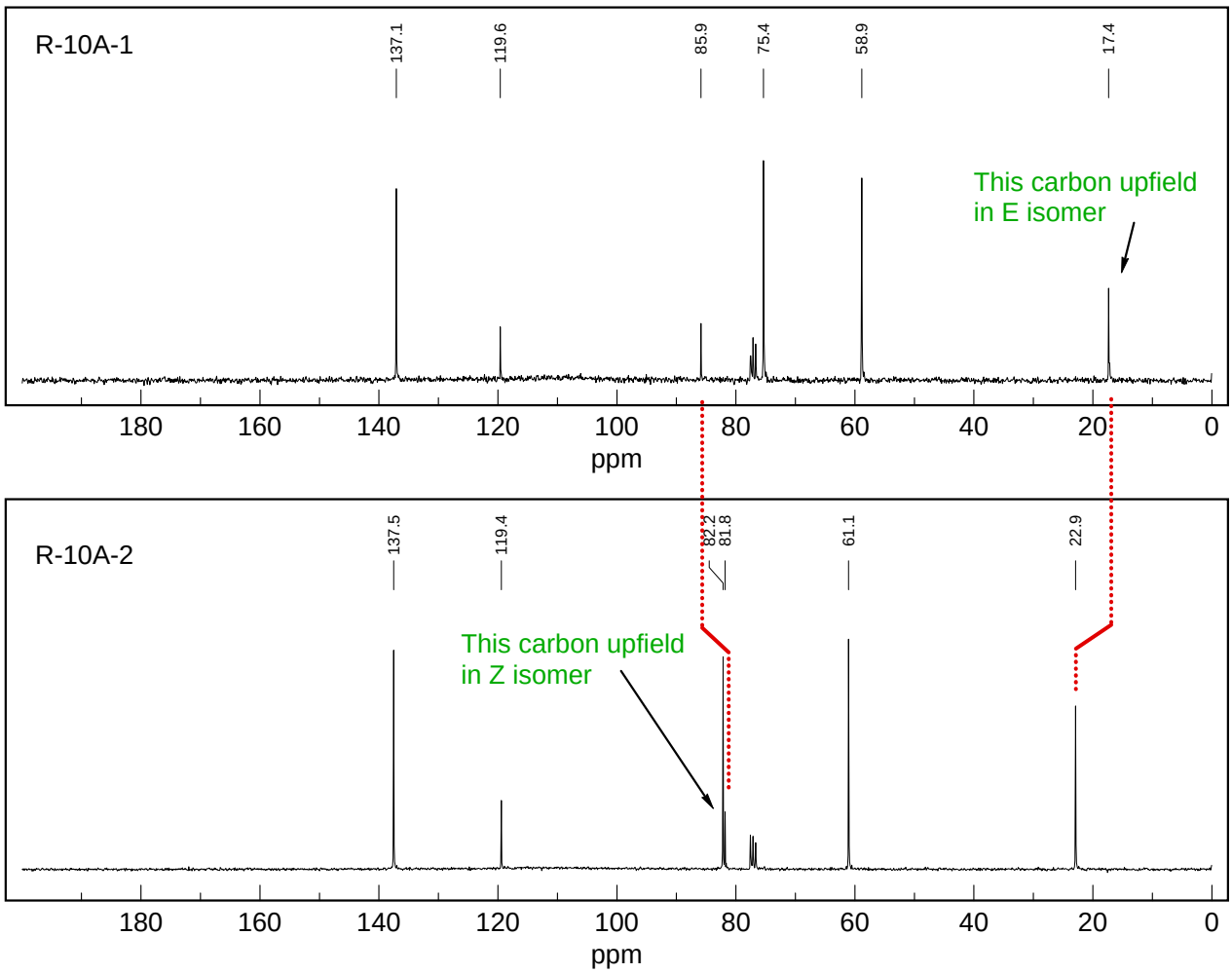
γ-effect, C≡C should be upfield (-4.1 ppm)



Z-isomer

R-10A-**2**

3



Briefly explain the basis for your assignment. Be specific.

4

γ-Interaction across double bonds causes upfield shifts (vs H at one of the positions). Thus in the E-isomer the CH_3 would be upfield ca 5 ppm compared to the Z-isomer. SImilarly, the first C≡C carbon would be upfield in the Z-isomer compared to the E

For some reason the terminal acetylene carbon also moves significantly (6.8 ppm) between isomers, but this is not a predictable γ-effect.