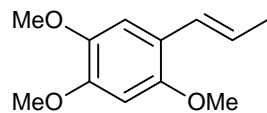
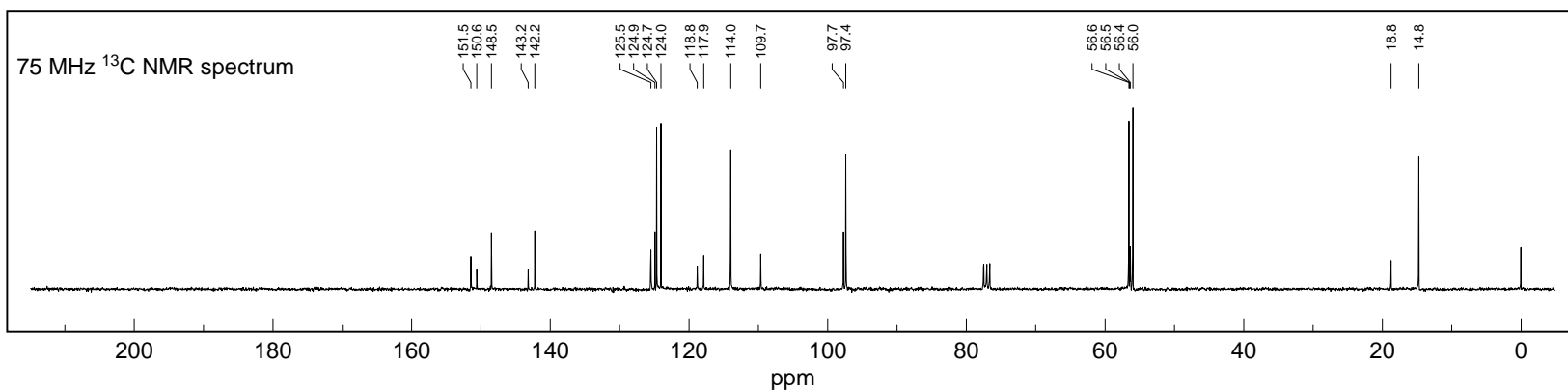
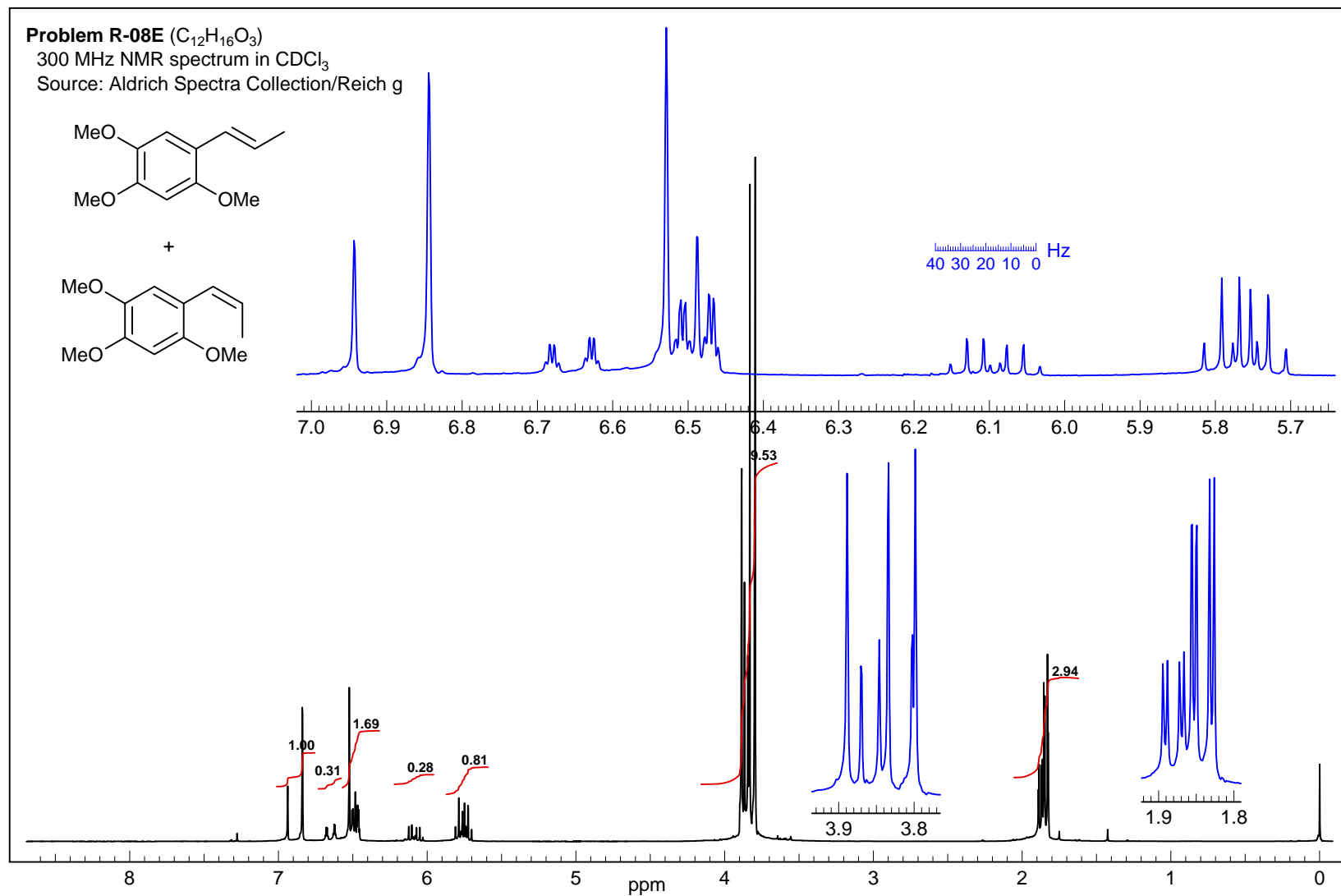
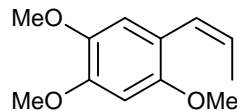


**Problem R-08E (C<sub>12</sub>H<sub>16</sub>O<sub>3</sub>)**300 MHz NMR spectrum in CDCl<sub>3</sub>

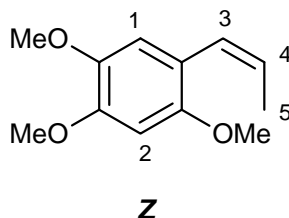
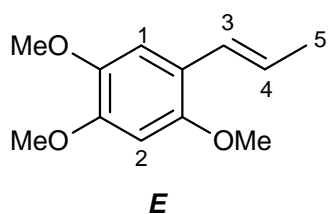
Source: Aldrich Spectra Collection/Reich g



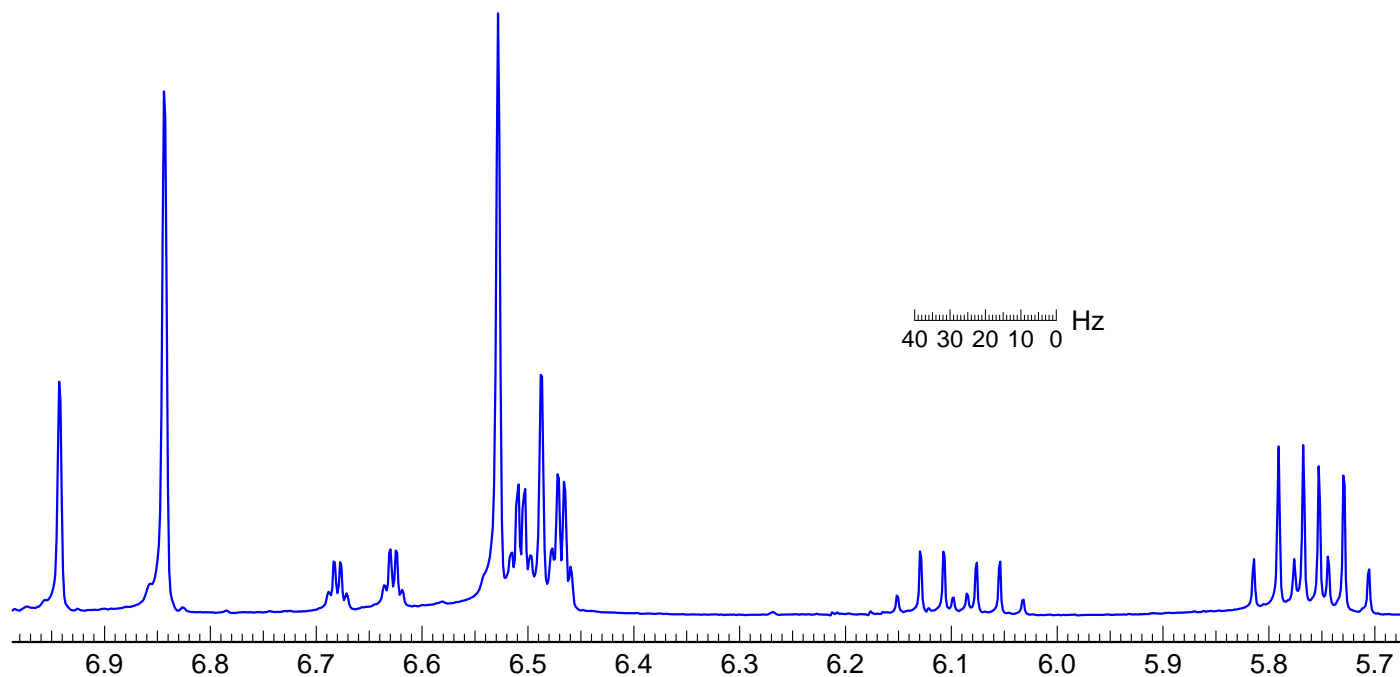
+



**Problem R-08E.** You are given the  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of a mixture of stereoisomers.



(a) Identify which is the major and which the minor isomer in the  $^1\text{H}$  NMR spectrum, and place assignments (E-1, E-2, Z-3, Z-4, etc.) over the appropriate peaks in the expansion below.

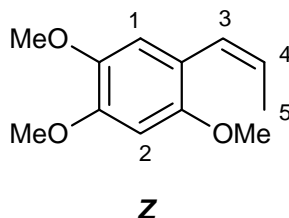
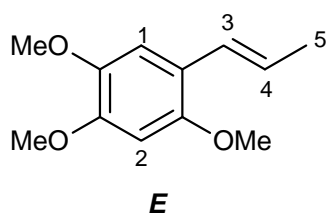


(b) Explain specifically how you made the E/Z assignment. Describe the multiplets you used (eg.  $J=7, 3$  Hz at  $\delta$  3.4) for each isomer.

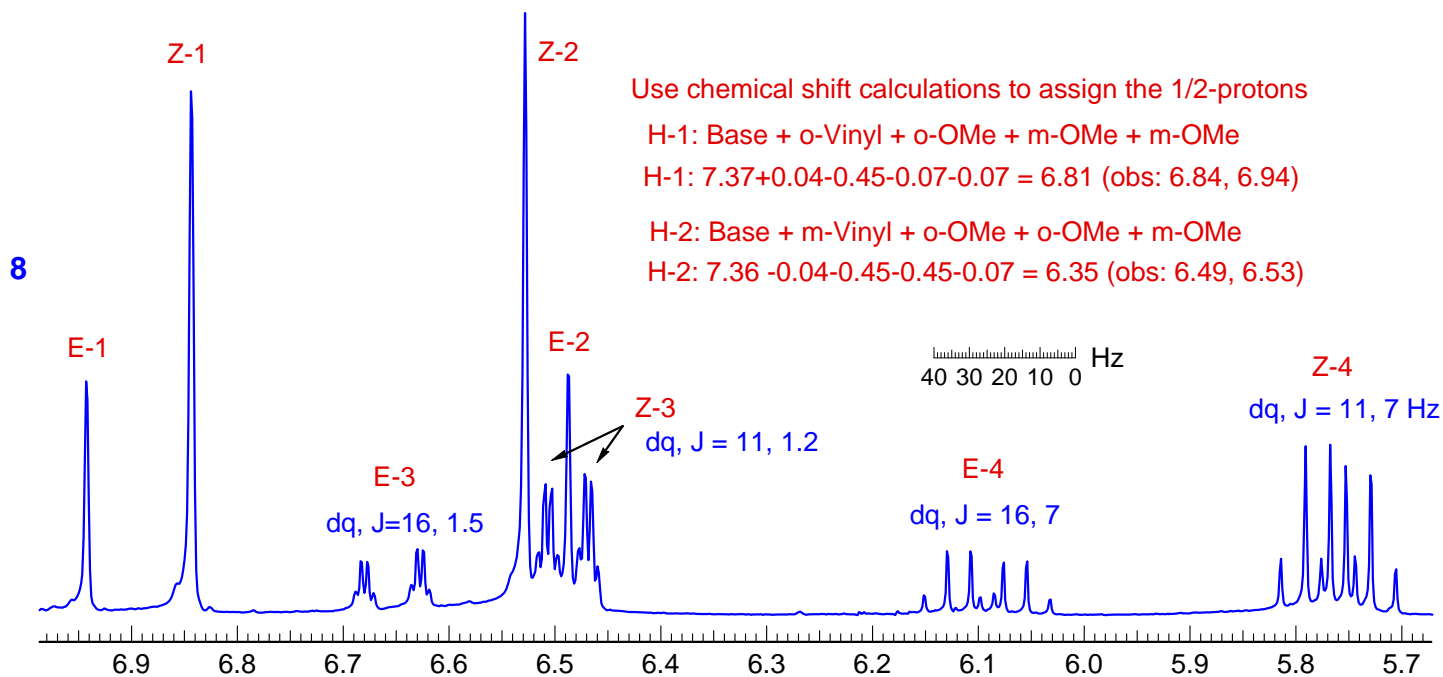
(c) Identify a feature of the  $^{13}\text{C}$  NMR spectrum which allows a firm structure assignment.

15

**Problem R-08E.** You are given the 300 MHz  $^1\text{H}$  NMR spectrum of a mixture of stereoisomers. The full spectrum is on the next page, but you only need to deal with the expansion on this page.



(a) Identify which is the major and which the minor isomer, and place assignments (E-1, E-2, Z-3, Z-4, etc.) over the appropriate peaks in the expansion below.



(b) Explain specifically how you made the E/Z assignment. Describe the multi-plets you used (eg.  $J=7, 3$  Hz at  $\delta$  3.4) for each isomer.

**7** The minor isomer has a dq,  $J = 16, 7$  at  $\delta$  6.09, and a dq,  $J=16, 1.5$  at  $\delta$  6.65, thus these protons are trans on the double bond

The major isomer has the corresponding coupling of 11 Hz ( $\delta$  5.76, dq,  $J = 11, 7$  Hz; 6.48, dq,  $J = 11, 1.2$  Hz)), thus the cis isomer

(c) Identify a feature of the  $^{13}\text{C}$  NMR spectrum which allows a firm structure assignment.

5

The  $\text{CH}_3$  carbons should show a substantial (several ppm) difference between the E and Z-isomers, with the Z-isomer upfield (cis gamma-effect). Indeed, the major isomer (Z) has the  $\text{CH}_3$  at  $\delta$  14.8, the minor at  $\delta$  18.8.