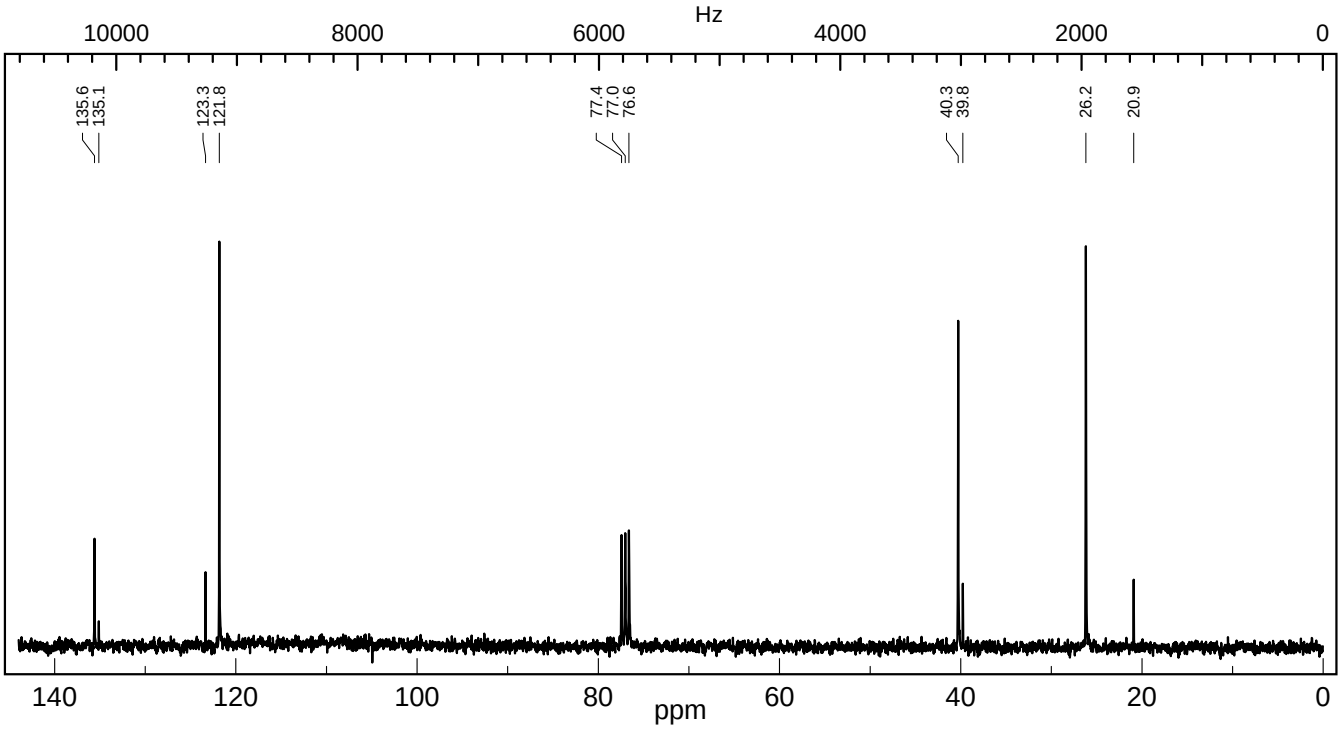
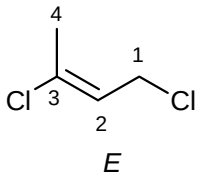
Problem R-96A ($C_4H_6Cl_2$) A 75 MHz ^{13}C NMR spectrum of an approximately 7:1 mixture of cis-trans isomers of 1,3-dichloro-2-butene is provided below. (Source: Aldrich Spectra Viewer, Solvent: $CDCl_3$).

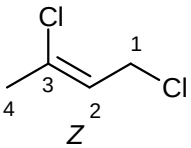


(a) Assign the individual carbons, and determine which is the major isomer.

	Assignment (*E* or *Z*: 1, 2, 3, or 4)
20.9	_____
26.2	_____
39.7	_____
40.2	_____
122.0	_____
123.6	_____
135.2	_____
135.6	_____



E



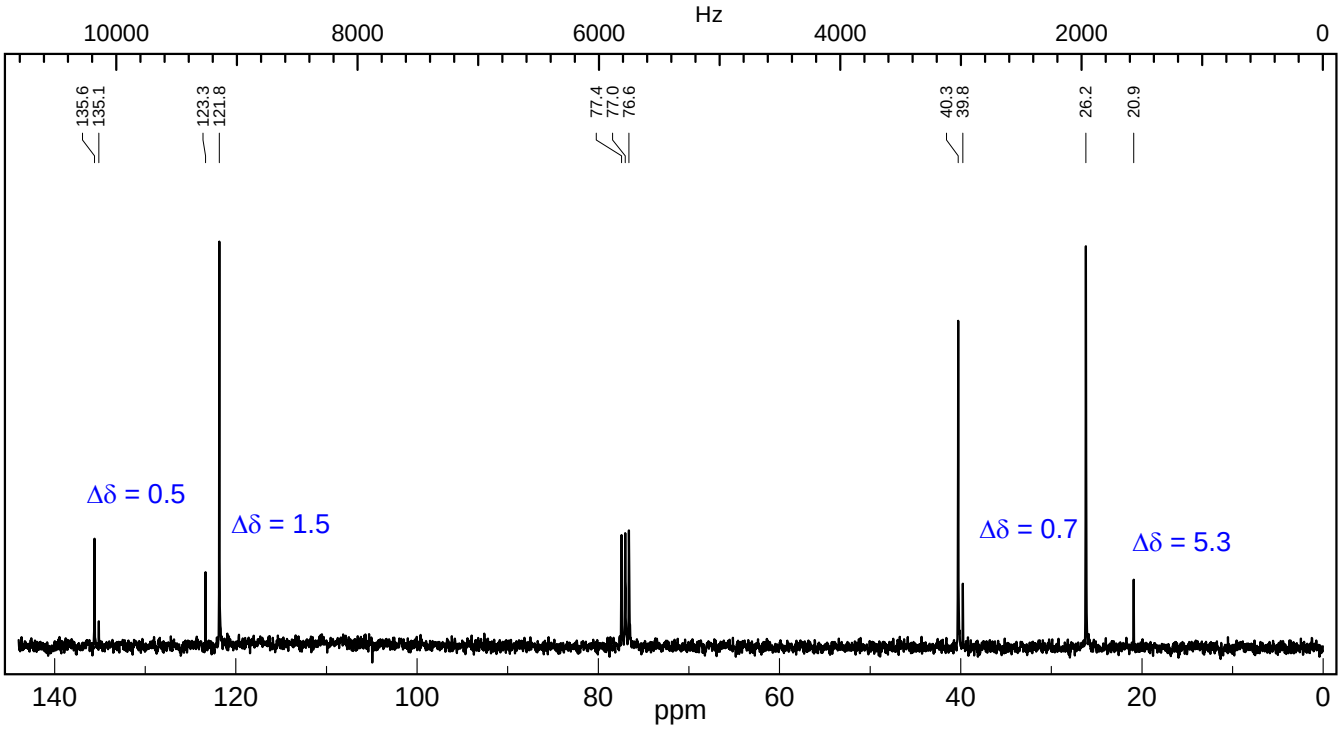
Z

(b) Explain clearly how you made the *E/Z* assignment (identify the signal(s) used).

(c) From the frequency and ppm scales, determine the spectrometer frequency (MHz):_____

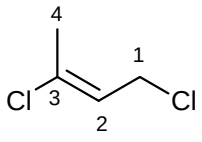
PLT ex-1-96-g.plt

Problem R-96A ($C_4H_6Cl_2$) A 75 MHz ^{13}C NMR spectrum of an approximately 7:1 mixture of cis-trans isomers of 1,3-dichloro-2-butene is provided below. (Source: Aldrich Spectra Viewer, Solvent: $CDCl_3$).

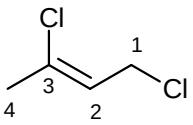


(a) Assign the individual carbons, and determine which is the major isomer.

	Assignment (*E* or *Z*: 1, 2, 3, or 4)
20.9	E-4
26.2	Z-4
39.7	E-1
40.2	Z-1
122.0	Z-2
123.6	E-2
135.2	E-3
135.6	Z-3



E



Z

(b) Explain clearly how you made the *E/Z* assignment (identify the signal(s) used).

Only the signals at δ 25, which can be assigned to C^4, have a significant difference in chemical shift in the two isomers - the other differences are probably too small to be useful.

C^4 should be upfield in the E isomer because of the cis-γ-effect - thus the small peak at 20.9 is the CH_3 (C^4) of the E-isomer, upfield of the Z isomer by 5.3 ppm.

C^1 sees a γ-effect in both isomers, although in the E isomer it is a Me and in the Z it is a Cl. Hard to predict which is bigger.

(c) From the frequency and ppm scales, determine the spectrometer frequency (MHz): 75 MHz

6000 Hz = 80 ppm 6000/80 = 75

PLT ex-1-96-g.plt