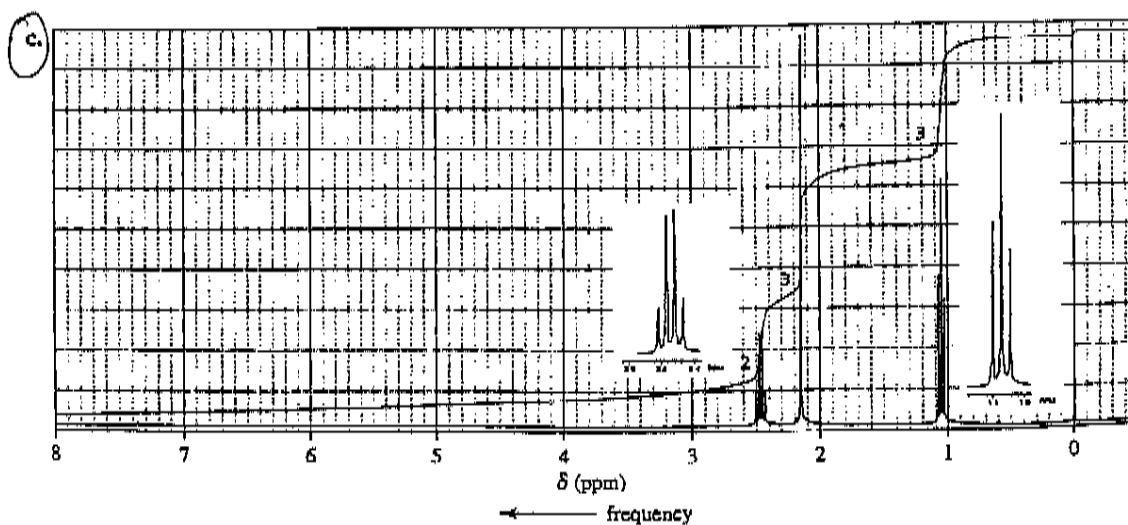
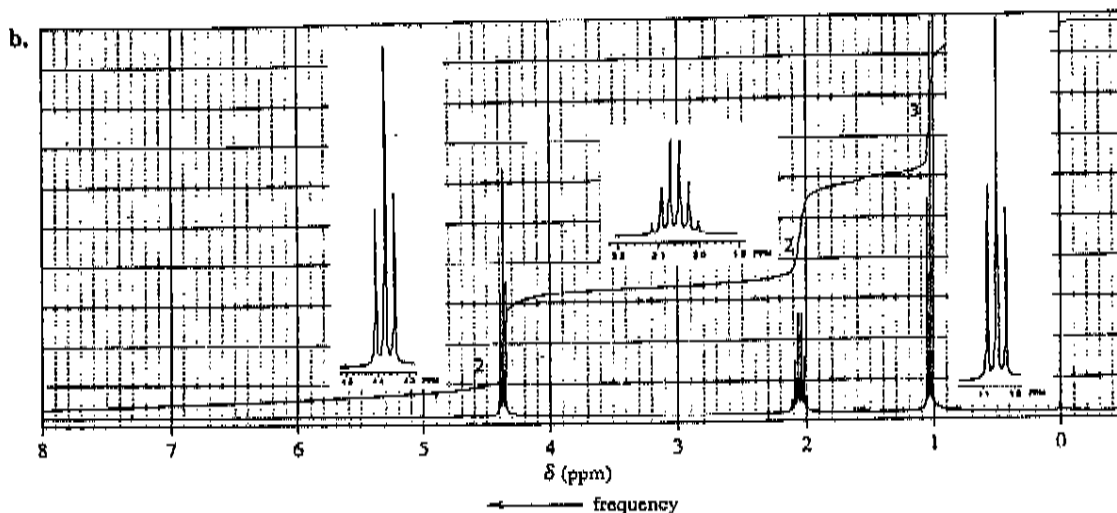
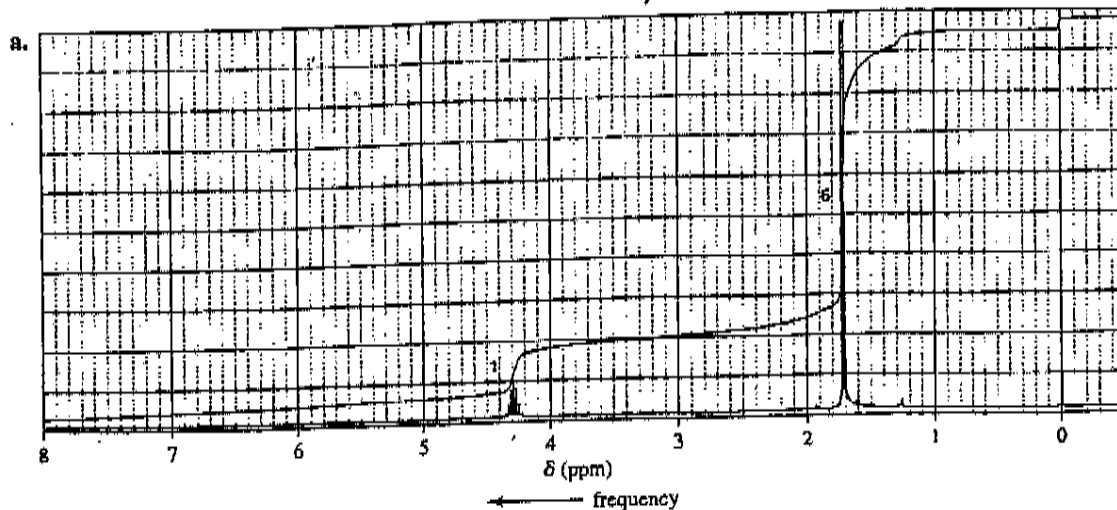
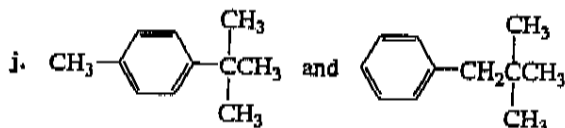
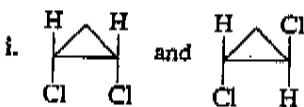
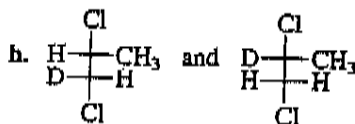
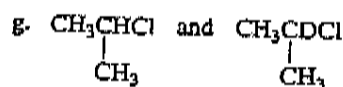
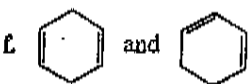
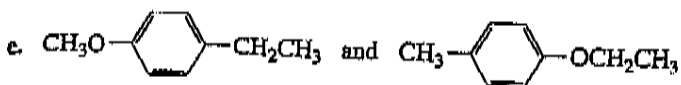
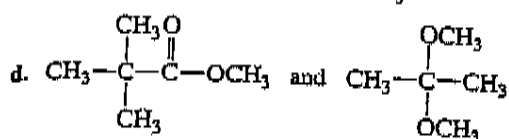
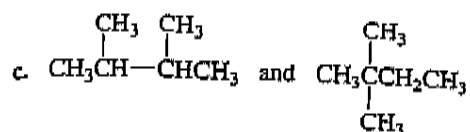


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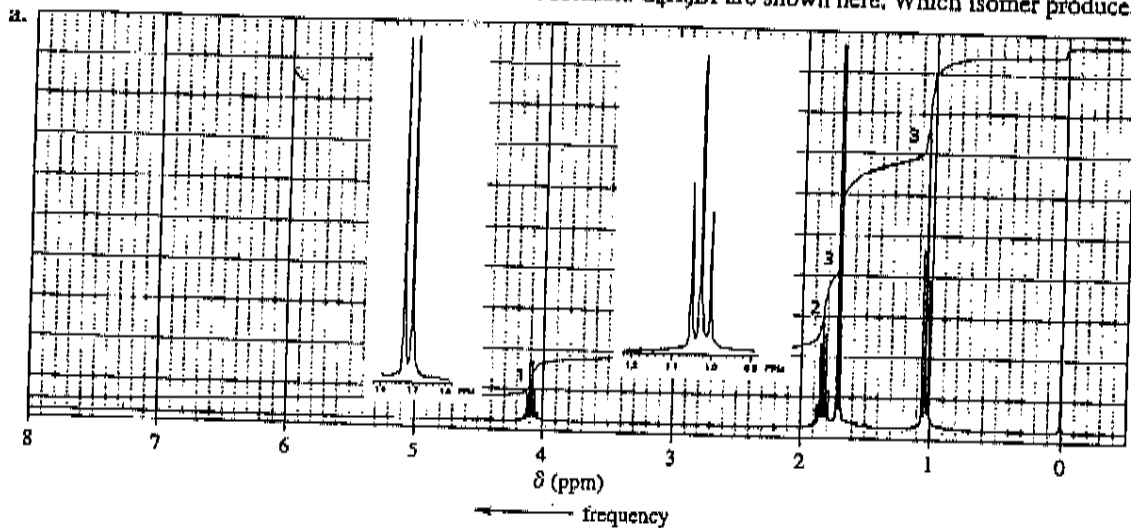
47. Determine the ratios of the chemically nonequivalent protons in a compound if the steps of the integration curves measure 40.5, 27.1, and 118 mm, from left to right across the spectrum. Give the structure of a compound whose  $^1H$  NMR spectrum would show these integrals in the observed order.
48. How could  $^1H$  NMR distinguish between the compounds in each of the following pairs?
- a.  $CH_3CH_2CH_2OCH_3$  and  $CH_3CH_2OCH_2CH_3$
- b.  $BrCH_2CH_2CH_2Br$  and  $BrCH_2CH_2CH_2NO_2$



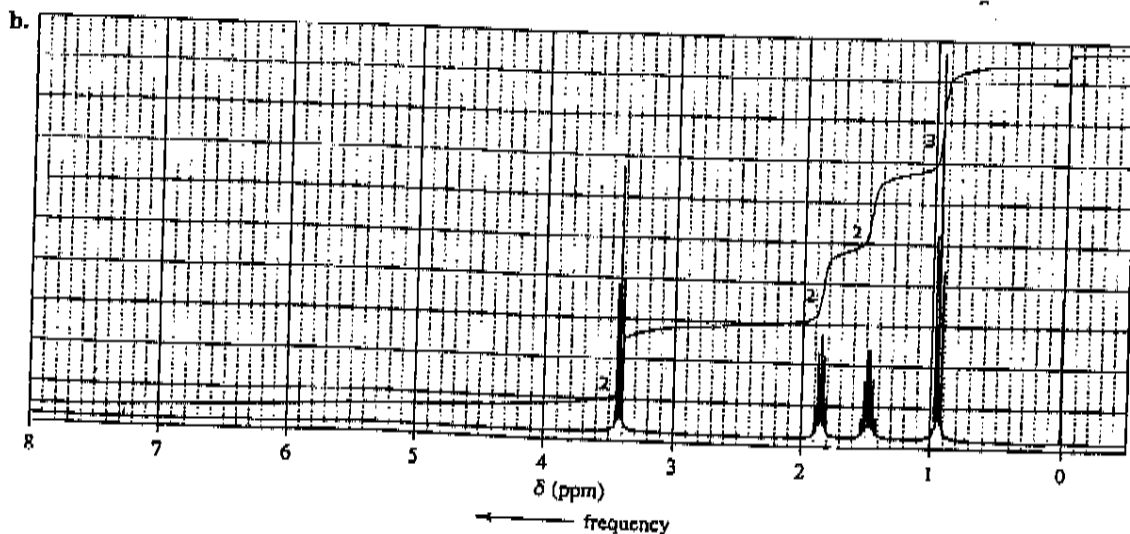
49. Answer the following questions:

- What is the relationship between chemical shift in ppm and operating frequency?
- What is the relationship between chemical shift in hertz and operating frequency?
- What is the relationship between coupling constant and operating frequency?
- How does the operating frequency in NMR spectroscopy compare with the operating frequency in IR and UV/Vis spectroscopy?

50. The  $^1\text{H}$  NMR spectra of three isomers with molecular formula  $\text{C}_4\text{H}_9\text{Br}$  are shown here. Which isomer produces which spectrum?

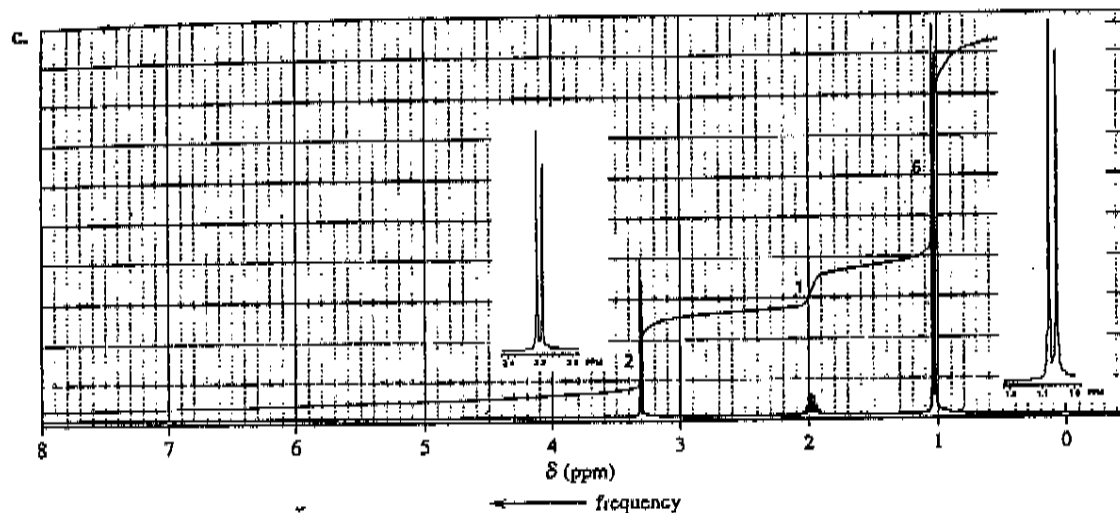


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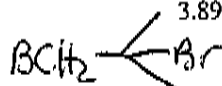
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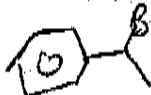
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51. Identify each of the following compounds from the  $^1\text{H}$  NMR data and molecular formula. The number of hydrogens responsible for each signal is shown in parentheses.

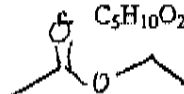
a.  $\text{C}_4\text{H}_8\text{Br}_2$  1.97 ppm (6) singlet  
3.89 ppm (2) singlet



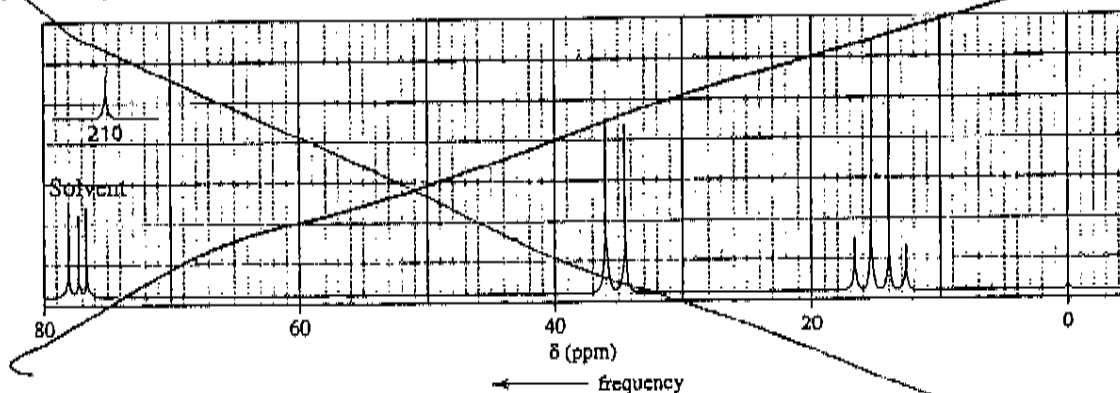
b.  $\text{C}_8\text{H}_9\text{Br}$  2.01 ppm (3) doublet  
5.14 ppm (1) quartet  
7.35 ppm (5) broad singlet



$\text{C}_5\text{H}_{10}\text{O}_2$  1.15 ppm (3) triplet  
1.25 ppm (3) triplet  
2.33 ppm (2) quartet  
4.13 ppm (2) quartet

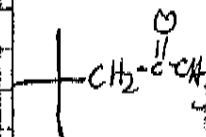
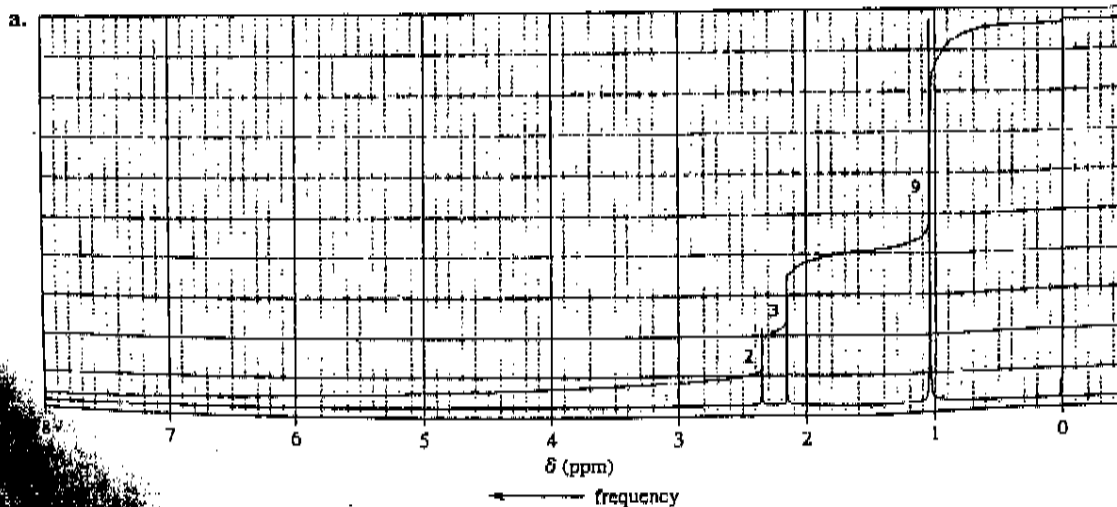


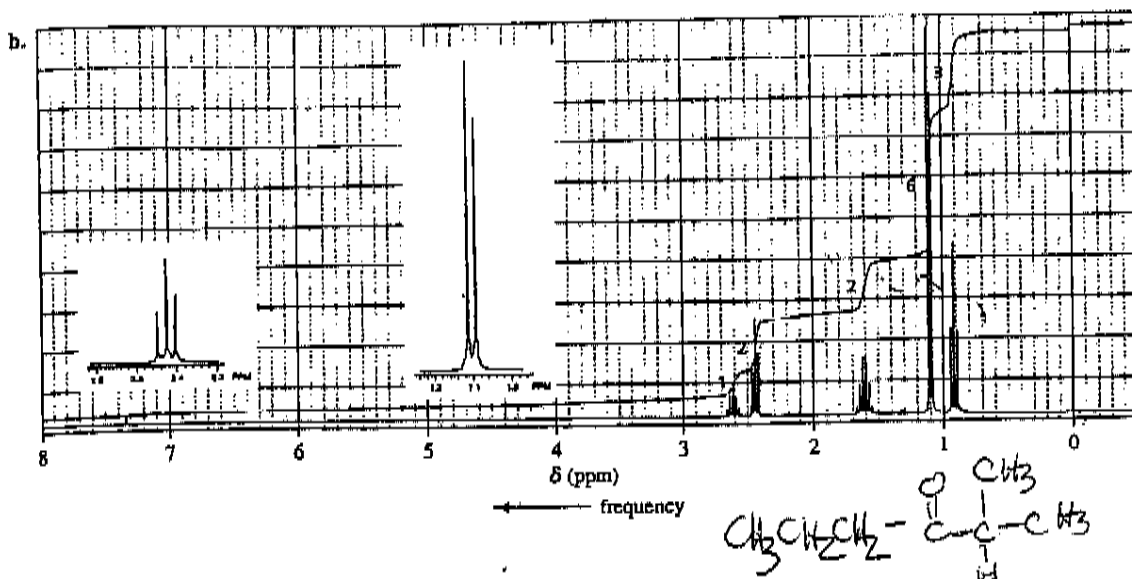
52. Identify the compound with molecular formula  $\text{C}_7\text{H}_{14}\text{O}$  that gives the following proton-coupled  $^{13}\text{C}$  NMR spectrum:



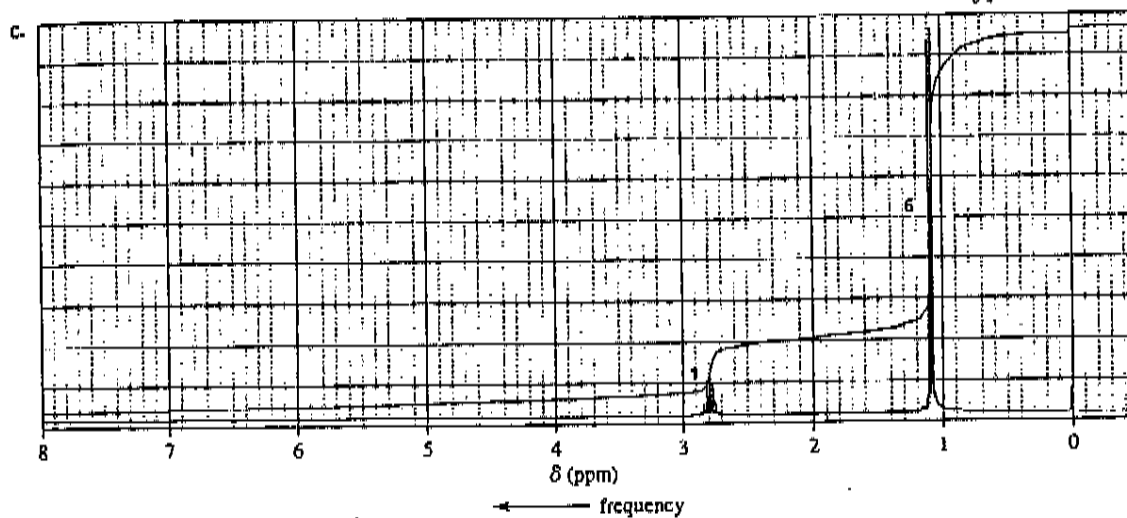
53. Compound A, with molecular formula  $\text{C}_4\text{H}_9\text{Cl}$ , shows two signals in its  $^{13}\text{C}$  NMR spectrum. Compound B, an isomer of compound A, shows four signals, and in the proton-coupled mode, the signal farthest downfield is a doublet. Identify compounds A and B.

54. The  $^1\text{H}$  NMR spectra of three isomers with molecular formula  $\text{C}_7\text{H}_{14}\text{O}$  are shown here. Which isomer produces which spectrum?





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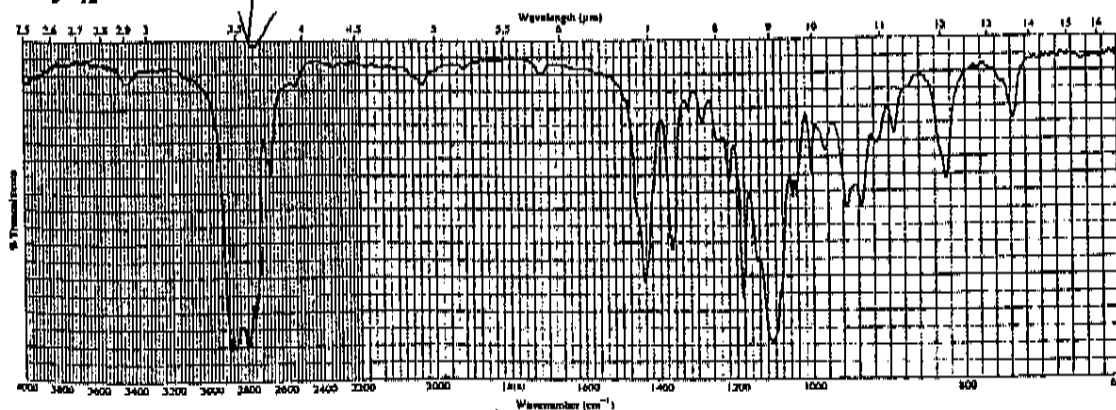


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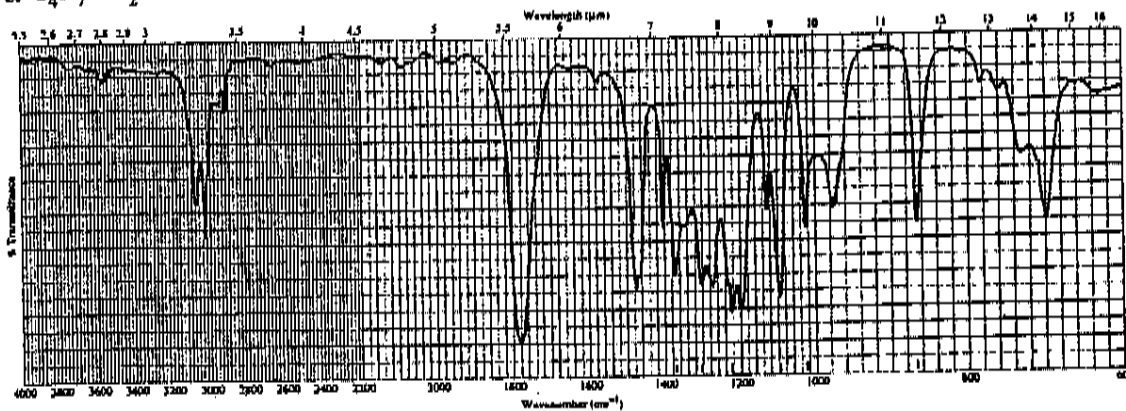
55. Would it be better to use  $^1\text{H}$  NMR or  $^{13}\text{C}$  NMR to distinguish between 1-butene, *cis*-2-butene, and 2-methylpropene? Explain your answer.

56. Determine the structure of each of the following unknown compounds based on its molecular formula and its IR and  $^1\text{H}$  NMR spectra.

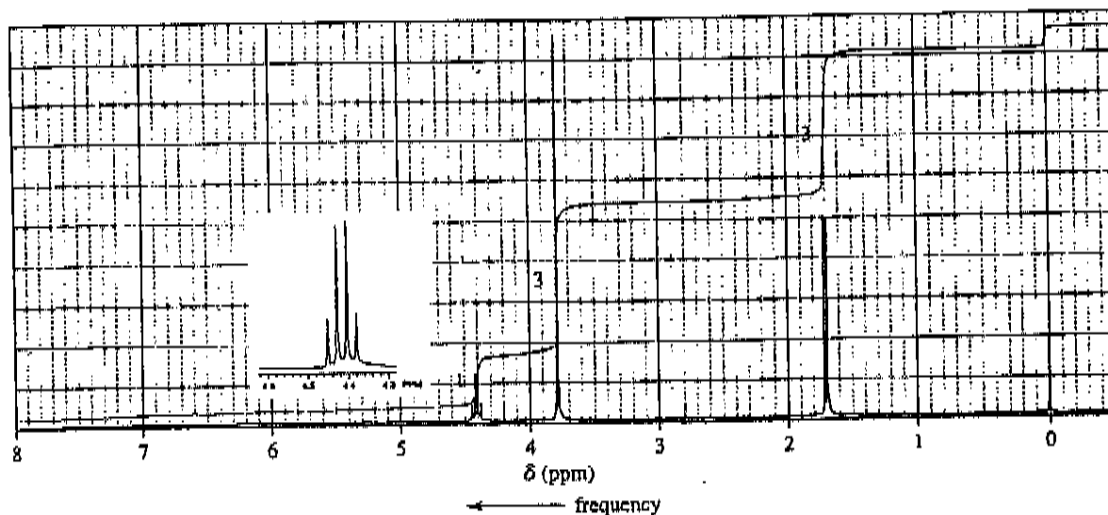
a.  $\text{C}_5\text{H}_{12}\text{O}$



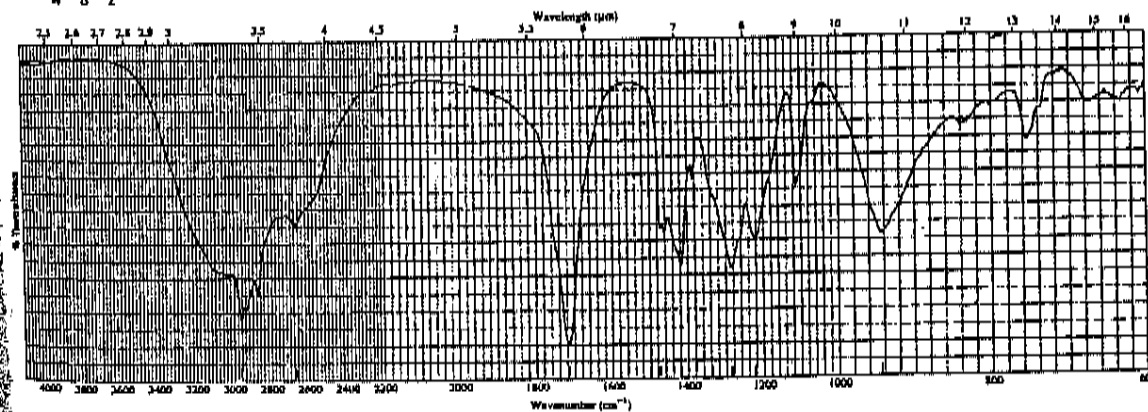
c.  $C_4H_7ClO_2$



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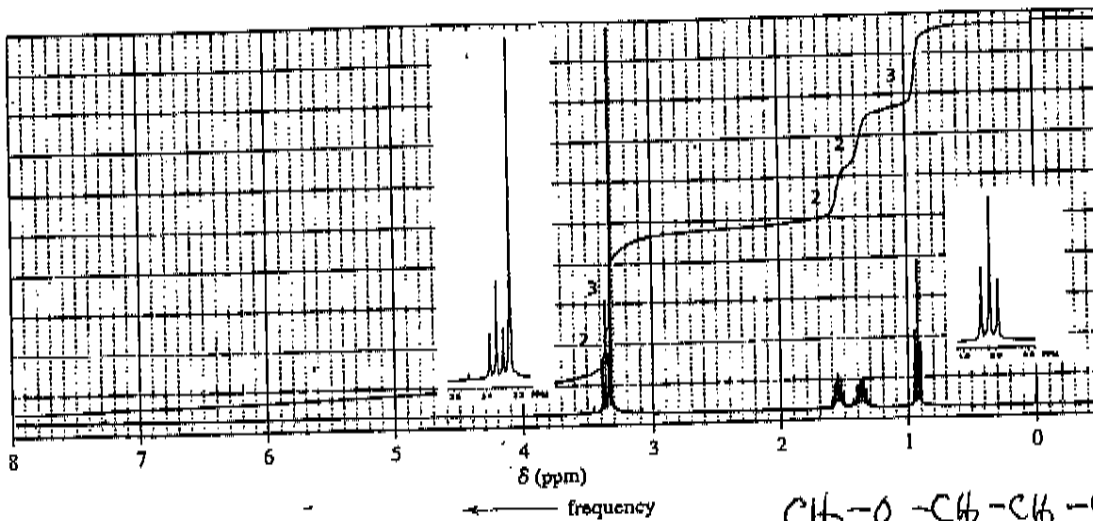


d.  $C_4H_8O_2$

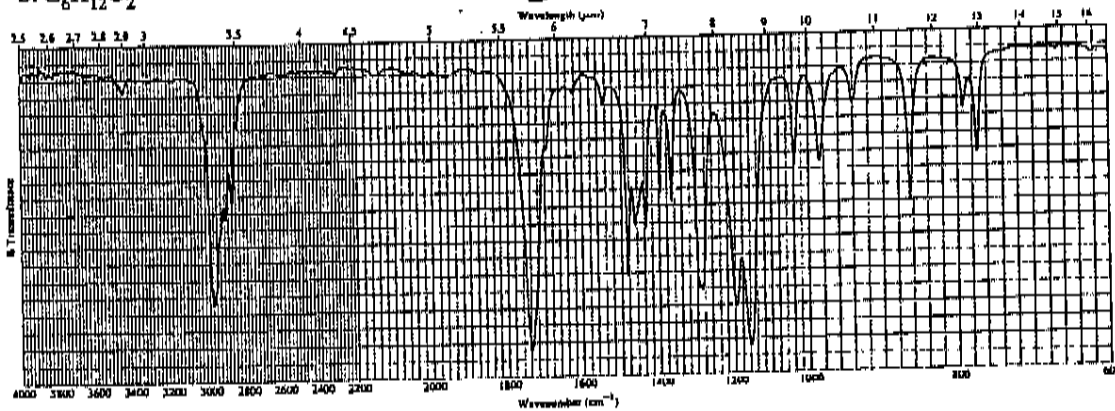


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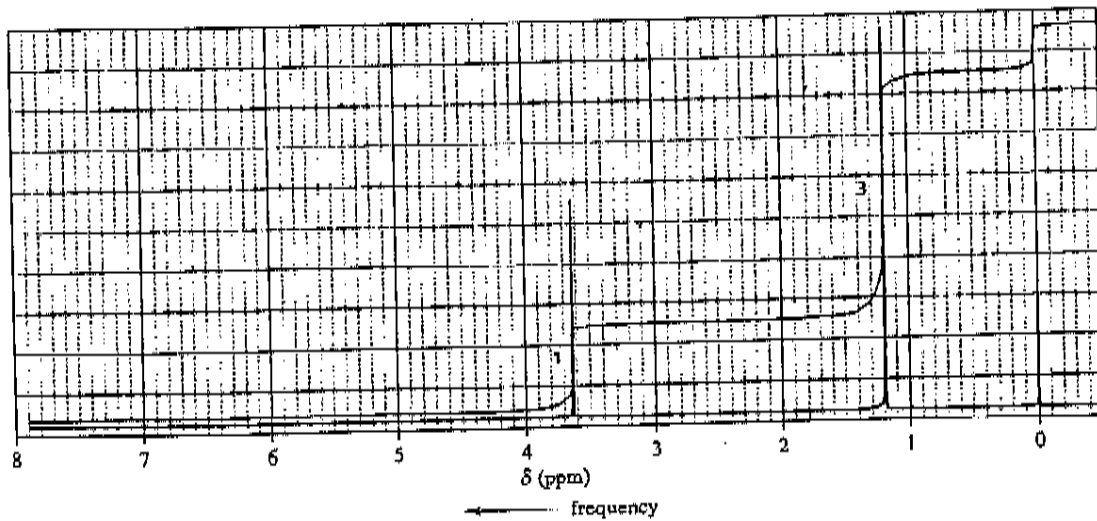
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b. C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>

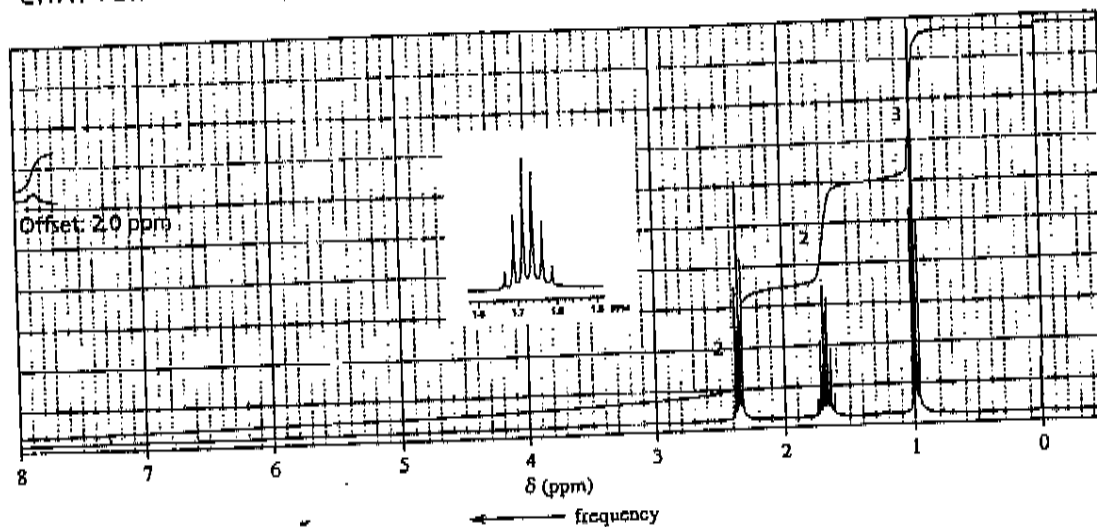


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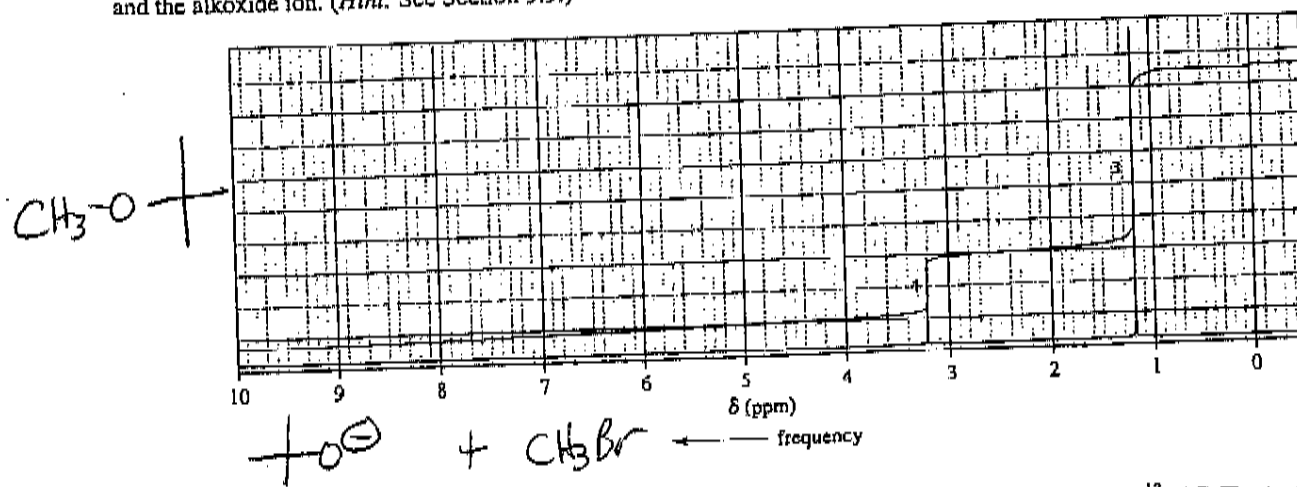


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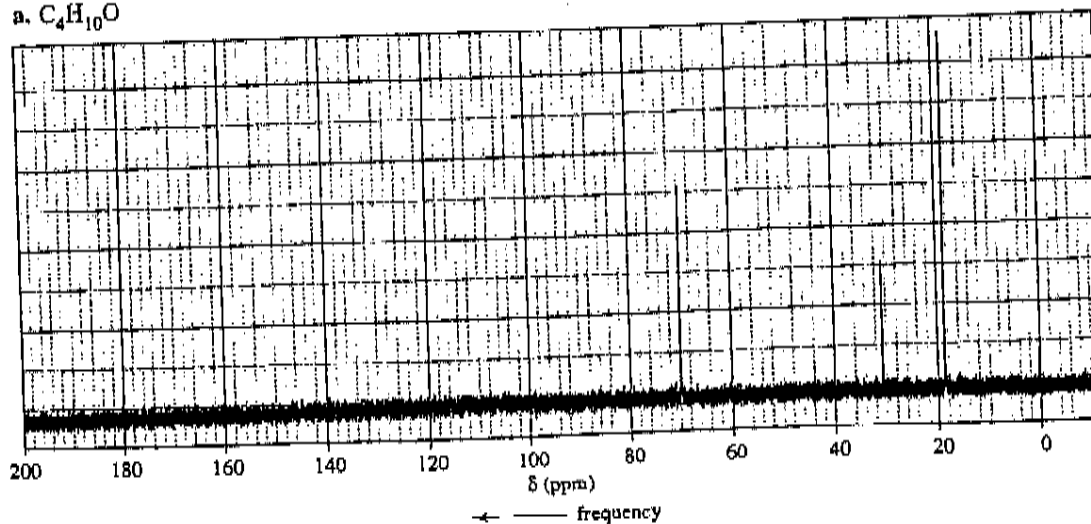


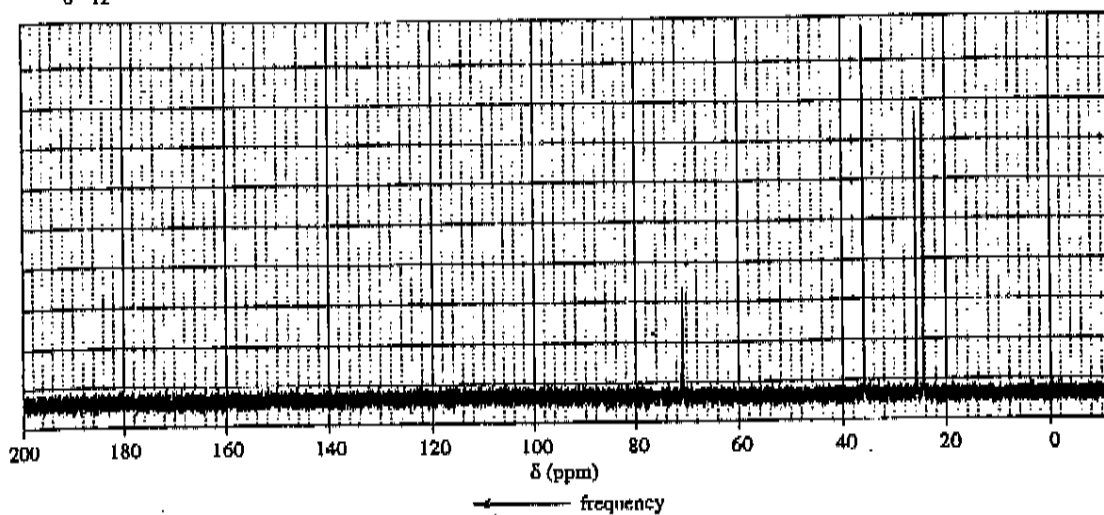
57. There are four esters with molecular formula  $C_4H_8O_2$ . How could they be distinguished by  $^1H$  NMR?
58. An alkyl halide reacts with an alkoxide ion to form a compound whose  $^1H$  NMR spectrum is shown here. Identify the alkyl halide and the alkoxide ion. (*Hint*: See Section 9.9.)



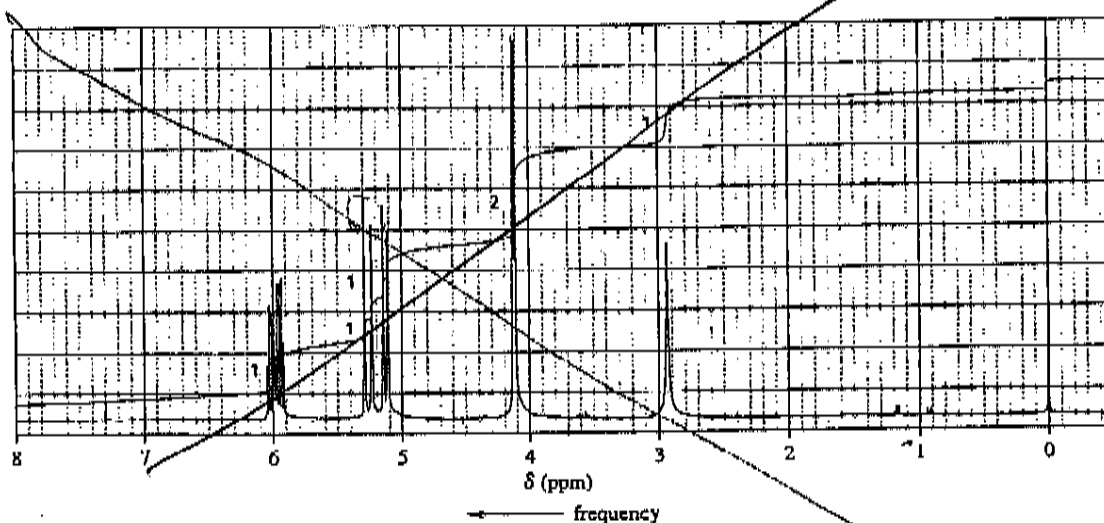
59. Determine the structure of each of the following compounds based on its molecular formula and its  $^{13}C$  NMR spectrum:

a.  $C_4H_{10}O$



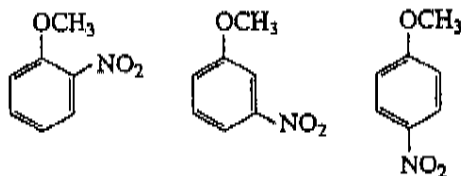
b.  $C_6H_{12}O$ 

60. The  $^1H$  NMR spectrum of 2-propen-1-ol is shown here. Indicate the protons in the molecule that give rise to each of the signals in the spectrum.



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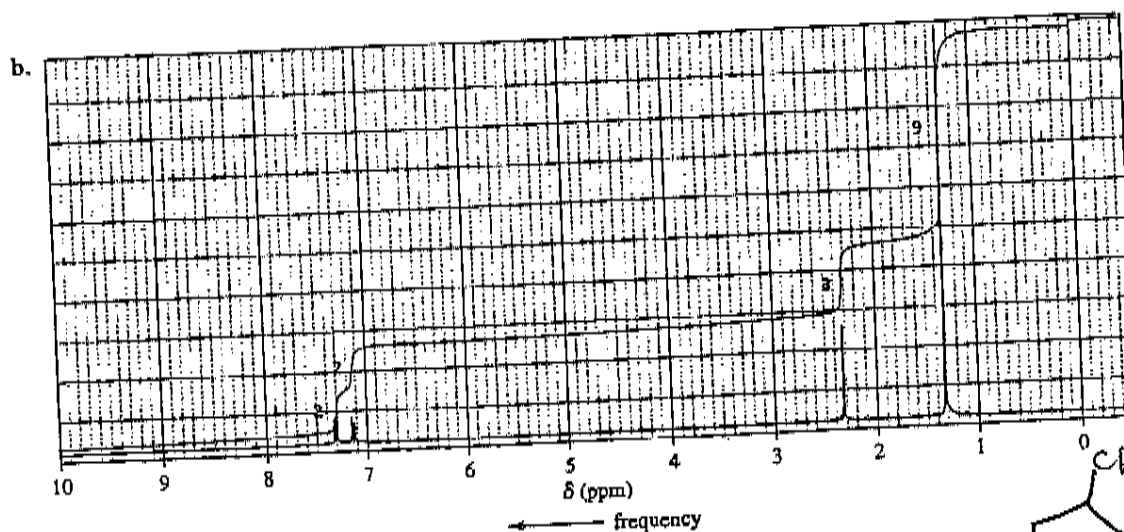
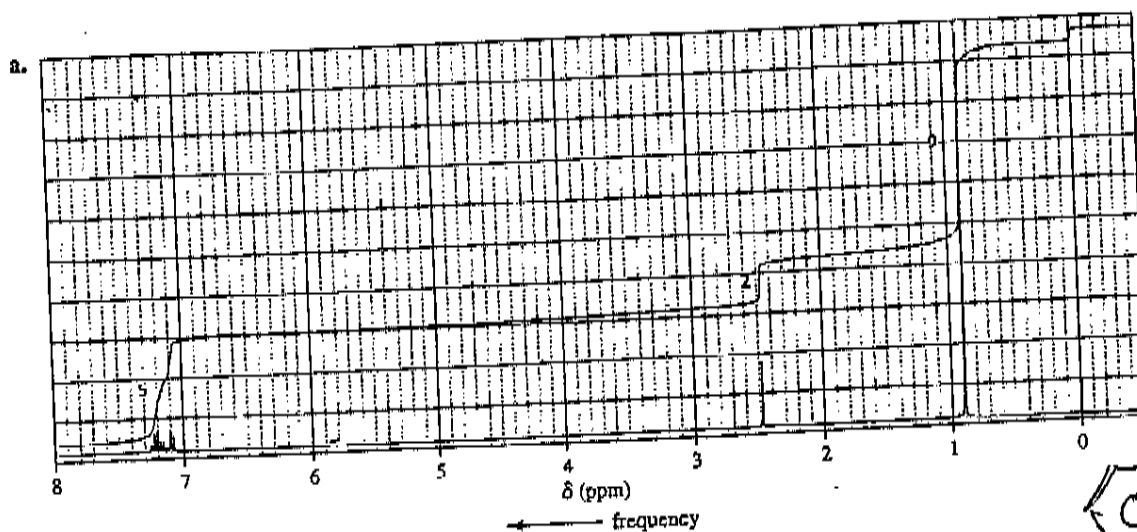
61. How could the signals in the 6.5 to 8.1-ppm region of their  $^1H$  NMR spectra distinguish between the following compounds?



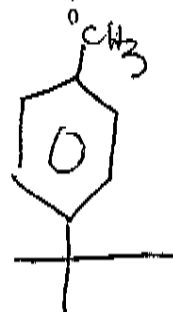
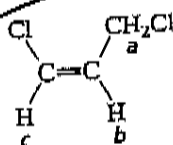


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62. The  $^1\text{H}$  NMR spectra of two compounds, each with molecular formula  $\text{C}_{11}\text{H}_{16}$ , are shown here. Identify the compounds.



63. Draw a splitting diagram for the  $\text{H}_b$  proton if  $J_{bc} = 10$  and  $J_{ba} = 5$ .

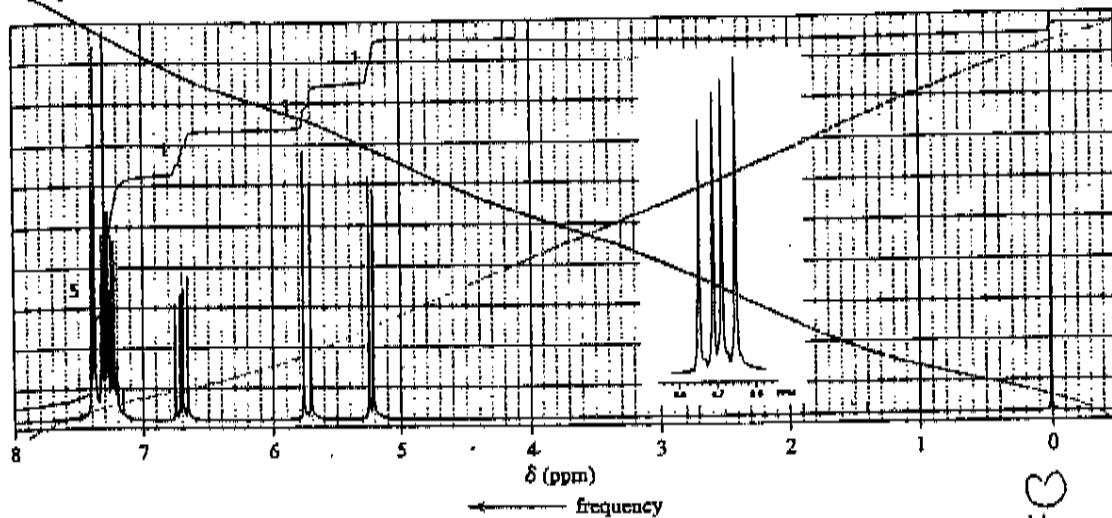


64. Sketch the following spectra that would be obtained for 2-chloroethanol:
- the  $^1\text{H}$  NMR spectrum for a dry sample of the alcohol.
  - the  $^1\text{H}$  NMR spectrum for a sample of the alcohol that contains a trace amount of acid.
  - the  $^{13}\text{C}$  NMR spectrum.
  - the proton-coupled  $^{13}\text{C}$  NMR spectrum.
  - the four parts of a DEPT  $^{13}\text{C}$  NMR spectrum.

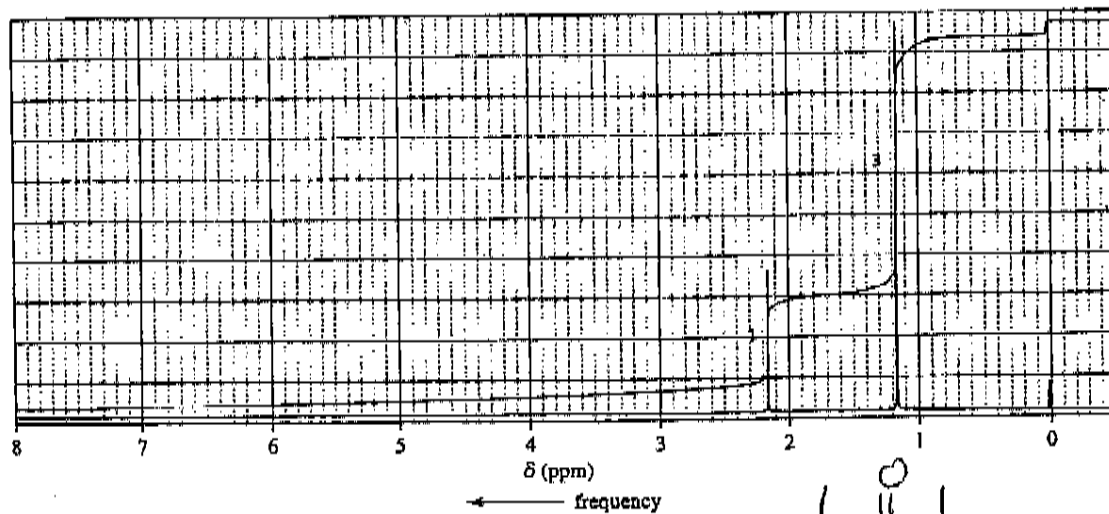
65. How could  $^1\text{H}$  NMR be used to prove that the addition of  $\text{HBr}$  to propene follows the rule that says that the electrophile adds to the  $\text{sp}^2$  carbon bonded to the greater number of hydrogens?

66. Identify each of the following compounds from its molecular formula and its  $^1\text{H}$  NMR spectrum.

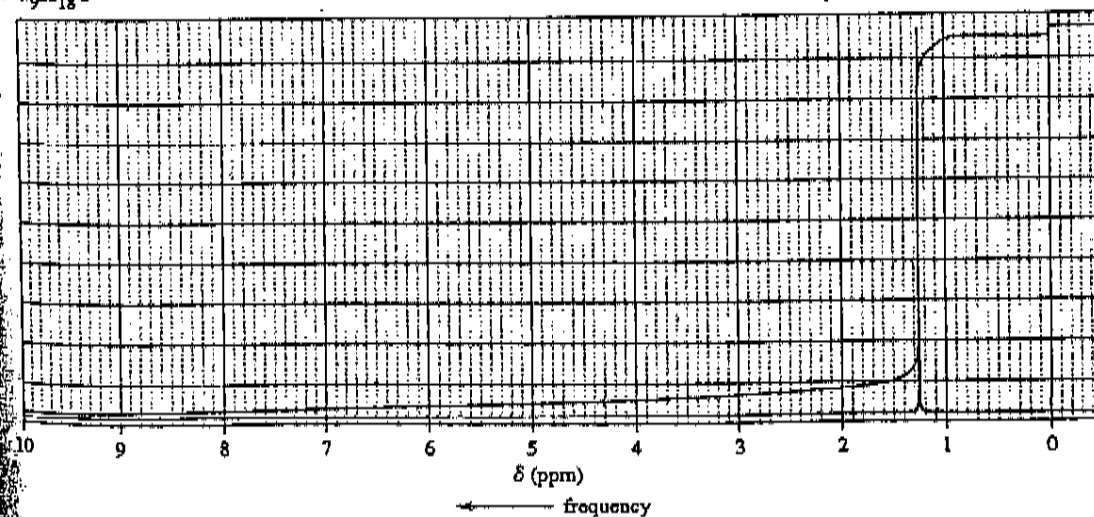
a.  $\text{C}_8\text{H}_8$



b.  $\text{C}_8\text{H}_{12}\text{O}$

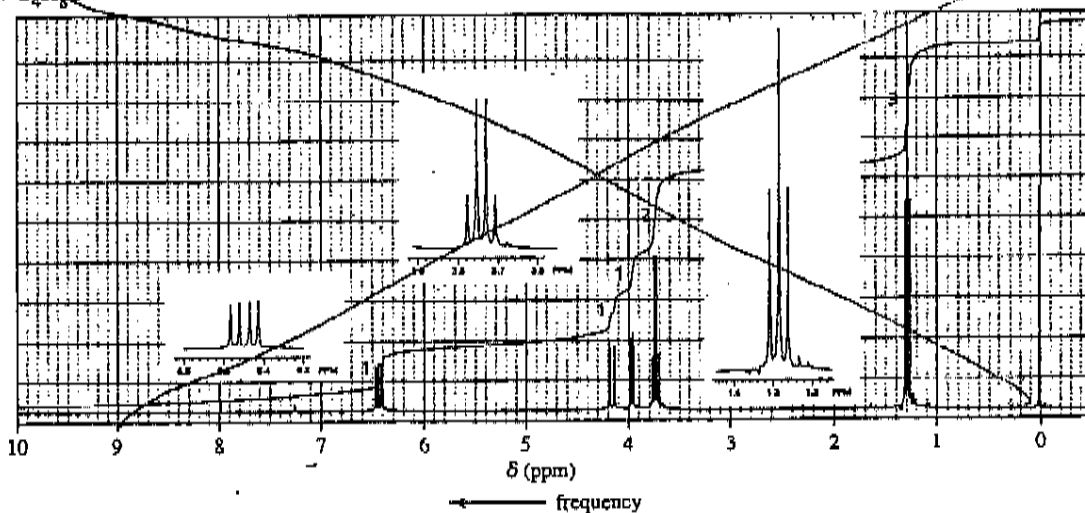


c.  $\text{C}_9\text{H}_{18}\text{O}$

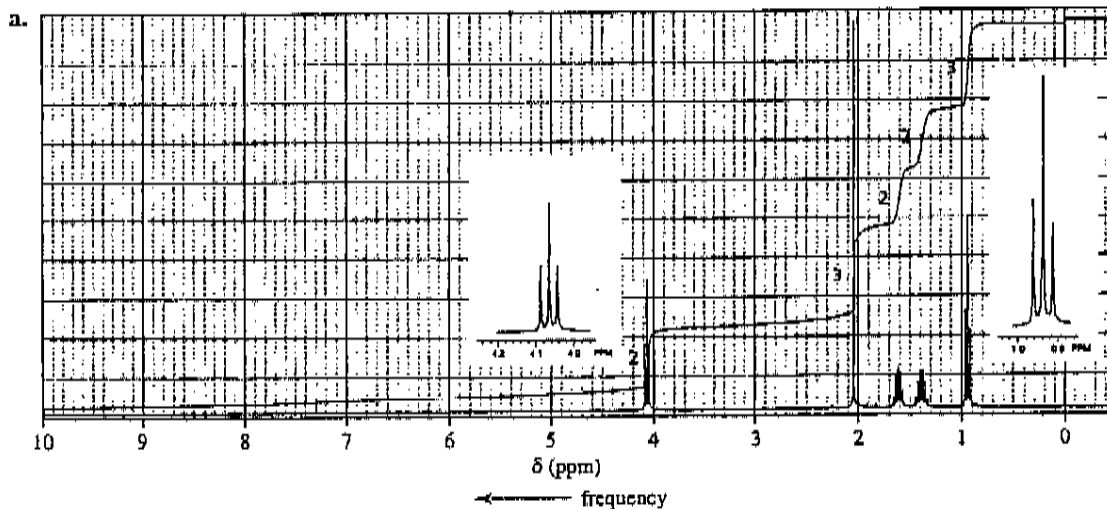


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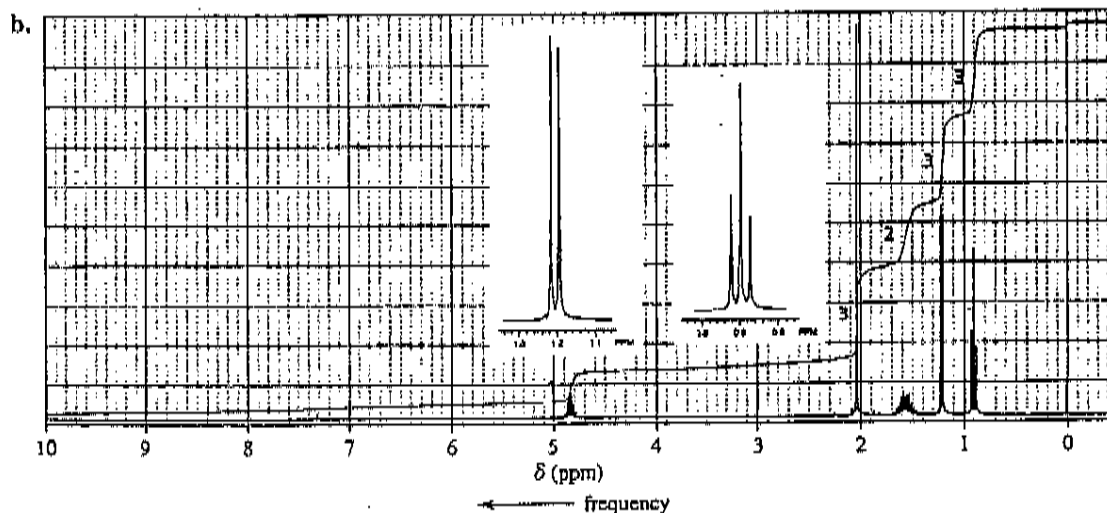
d.  $C_4H_8O$



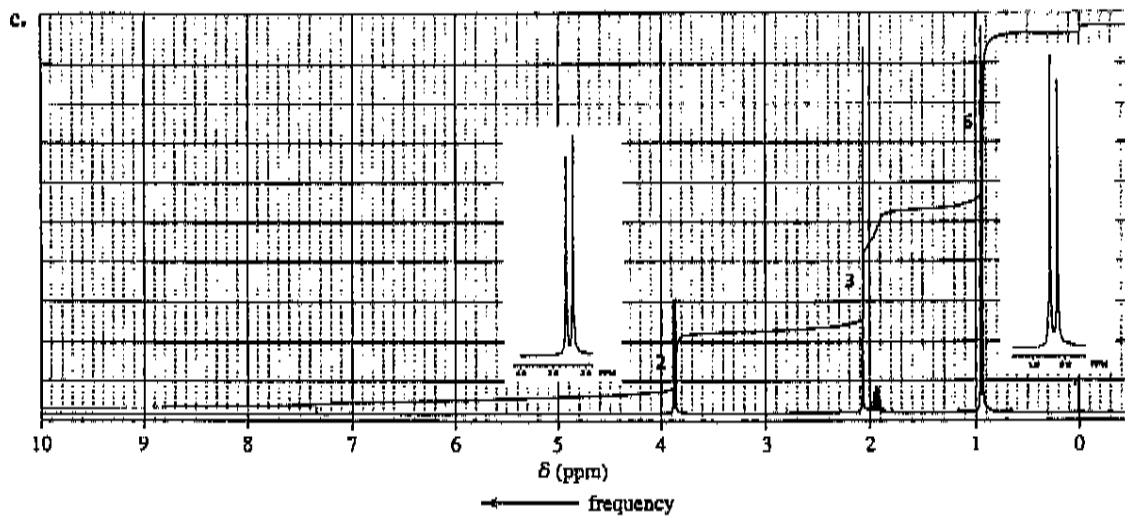
67. Dr. N. M. Arr was called in to help analyze the  $^1H$  NMR spectrum of a mixture of compounds known to contain only C, H, and Br. The mixture showed two singlets—one at 1.8 ppm and the other at 2.7 ppm—with relative integrals of 1 : 6, respectively. Dr. Arr determined that the spectrum was that of a mixture of bromomethane and 2-bromo-2-methylpropane. What was the ratio of bromomethane to 2-bromo-2-methylpropane in the mixture?
68. Calculate the amount of energy (in calories) required to flip an  $^1H$  nucleus in an NMR spectrometer that operates at 60 MHz.
69. The following  $^1H$  NMR spectra are for four compounds each with molecular formula  $C_6H_{12}O_2$ . Identify the compounds.



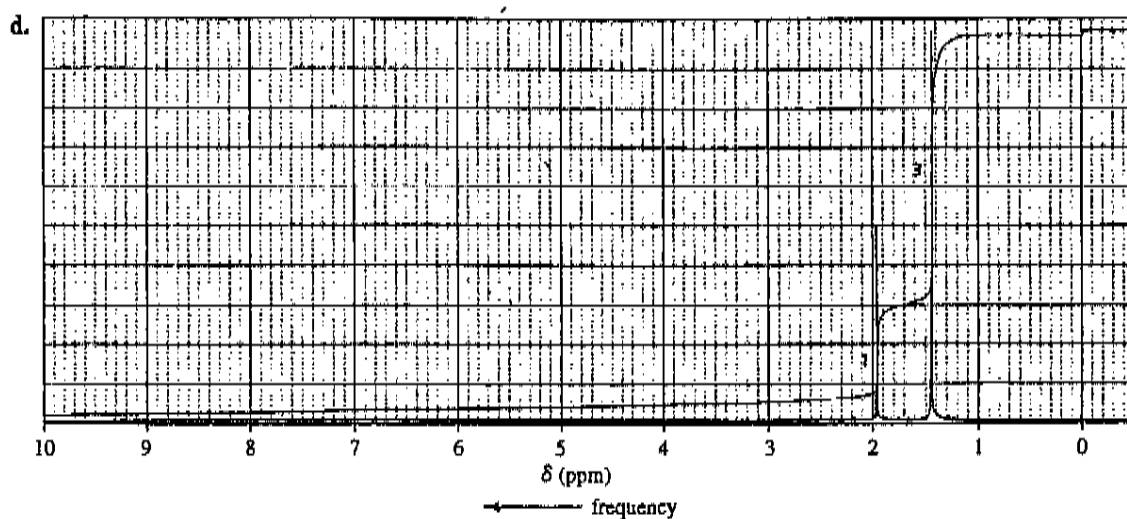
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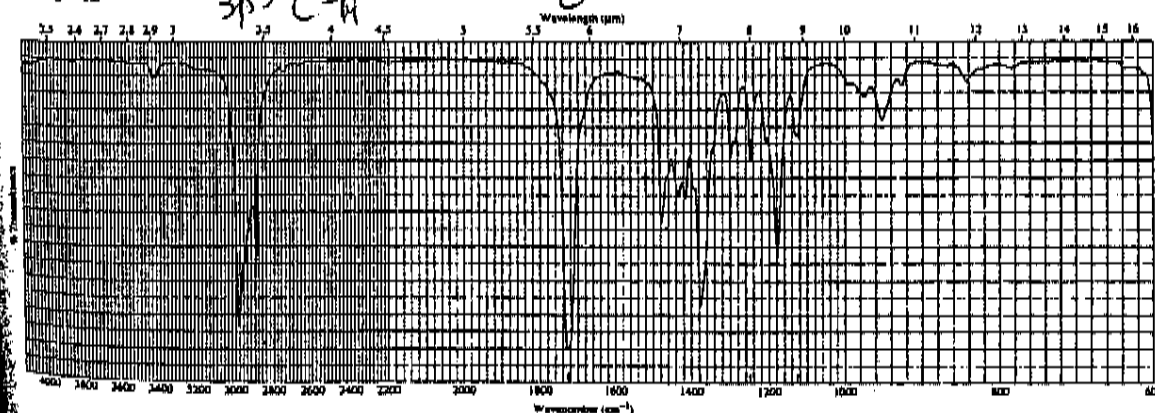


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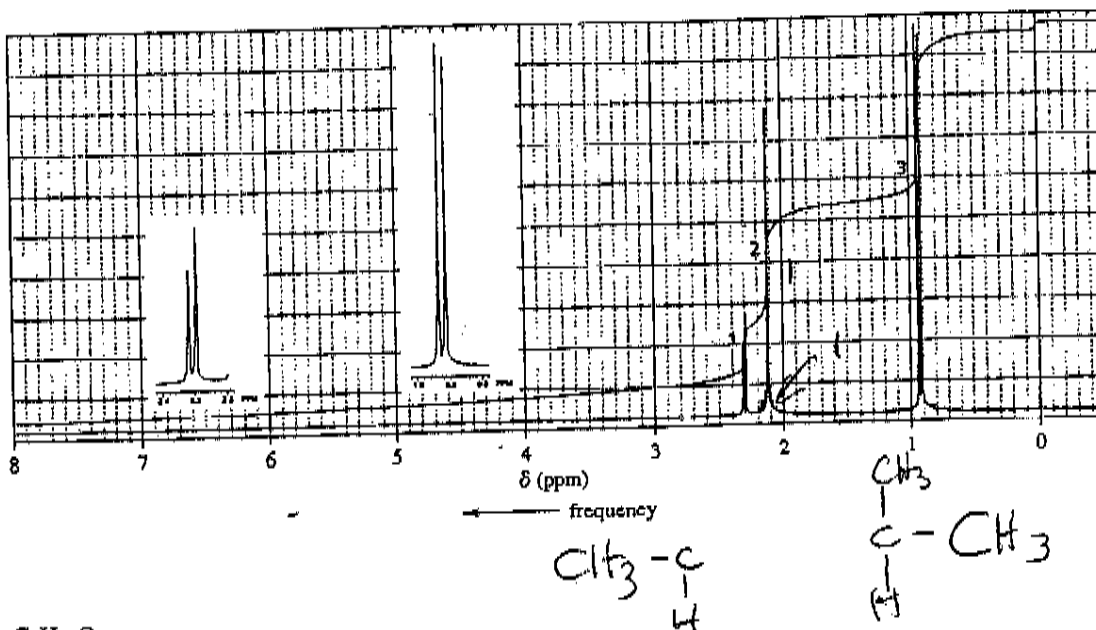
70. When compound A ( $C_5H_{12}O$ ) is treated with HBr, it forms compound B ( $C_5H_{11}Br$ ). The  $^1H$  NMR spectrum of compound A has one singlet (1), two doublets (3, 6), and two multiplets (both 1). (The relative areas of the signals are indicated in parentheses.) The  $^1H$  NMR spectrum of compound B has a singlet (6), a triplet (3), and a quartet (2). Identify compounds A and B.

71. Determine the structure of each of the following compounds, based on its molecular formula and its IR and  $^1H$  NMR spectra.

a.  $C_6H_{12}O$



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b.  $\text{C}_6\text{H}_{14}\text{O}$

