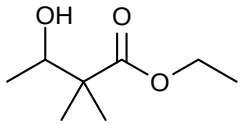
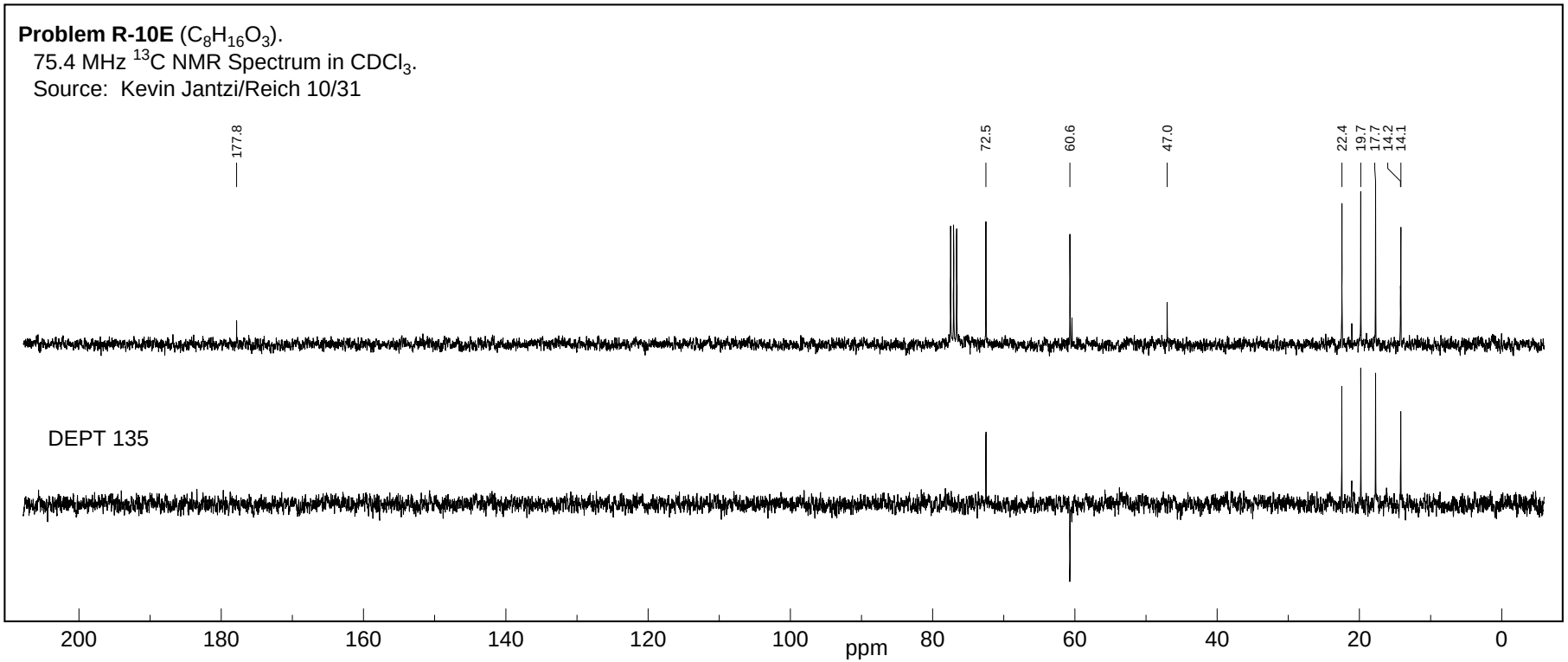
Problem R-10E ($C_8H_{16}O_3$).
300 MHz ^{1}H NMR Spectrum in $CDCl_3$.
Source: Joe Langenhan/Gellman 10/31 g

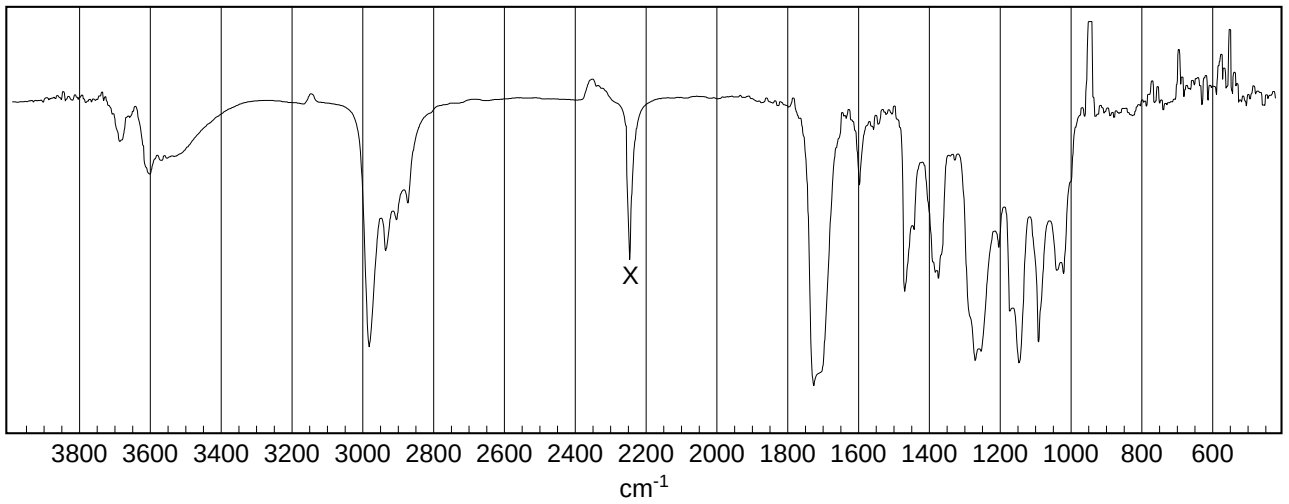


PLT ex-1-2010-11-gq.plt

Problem R-10E ($C_8H_{16}O_3$).
75.4 MHz ^{13}C NMR Spectrum in $CDCl_3$.
Source: Kevin Jantzi/Reich 10/31



Problem R-10E ($C_8H_{16}O_3$).
IR Spectrum Neat
Source: Nicolet FT-IR



PLT ex-1-2010-11-gq.plt

30 **Problem R-10E** ($C_8H_{16}O_3$). Determine the structure of **R-10E** from the ^{1}H NMR, ^{13}C NMR and IR spectra provided.

(a) DBE_____ (b) What information can you obtain from the IR spectrum (give frequency and peak assignment).

(c) Interpret the ^{13}C NMR spectrum, showing any part structures that can be identified, and the corresponding δ values.

δ
14.13
17.68
19.76
22.40
46.98
60.65
72.47
177.80

(d) The signal at δ 2.7 in the ^{1}H NMR spectrum disappears when the sample is shaken with D_2O, and the signal δ 3.9 becomes a 1:3:3:1 quartet. What does this tell you about the structure?

(e) Analyze the ^{1}H NMR spectrum. For each of the groups of signals marked on the spectrum, report the multiplet structure in the standard format (e.g., 0.0 δ, dtd, J = 0.0, 0.0, 0.0 Hz, 2H) and any part structure you could obtain from the signal(s).

A _____

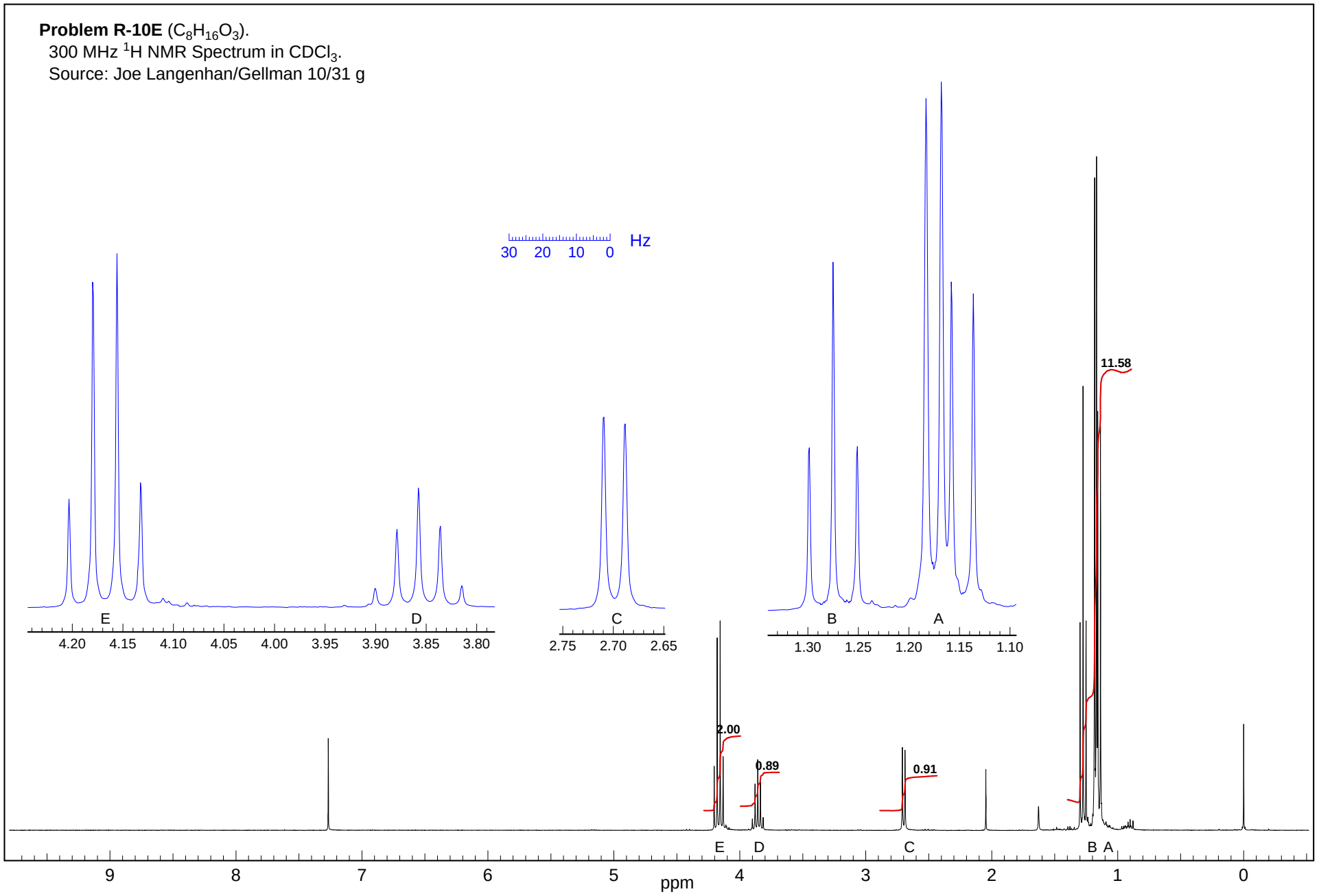
B _____

C _____

D _____

E _____

(f) Give your answer below. If more than one structure fits the data, draw them, but indicate your best choice by circling the structure



PLT ex-1-2010-11-gq.plt

30

Problem R-10E ($C_8H_{16}O_3$). Determine the structure of **R-10E** from the ^{1}H NMR, ^{13}C NMR and IR spectra provided.

(a) DBE 1 (b) What information can you obtain from the IR spectrum (give frequency and peak assignment).

3500-3600 cm^{-1} OH stretch 1730 cm^{-1} Carbonyl stretch - probably an ester

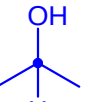
(c) Interpret the ^{13}C NMR spectrum, showing any part structures that can be identified, and the corresponding δ values.

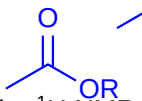
δ

14.13
17.68
19.76
22.40 — Very likely 4 CH_3

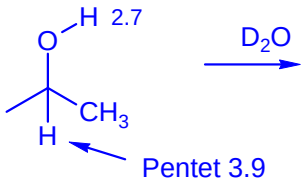
46.98 — 4* carbon (not bearing an O) disappears in DEPT

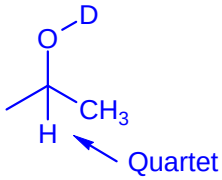
60.65 — must be $-CH_2-OR$

72.47 — Must be a 

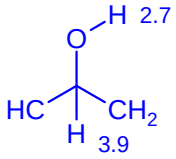
177.80 

(d) The signal at δ 2.7 in the ^{1}H NMR spectrum disappears when the sample is shaken with D_2O, and the signal δ 3.9 becomes a 1:3:3:1 quartet. What does this tell you about the structure?





Also possible:



4

(e) Analyze the ^{1}H NMR spectrum. For each of the groups of signals marked on the spectrum, report the multiplet structure in the standard format (e.g., 0.0 δ, dtd, J = 0.0, 0.0, 0.0 Hz, 2H) and any **part structure** you could obtain from the signal(s).

δ 1.15, 1H, d, J = 7Hz CH_3-C(H)

A δ 1.17, 1.18 - possible two methyl singlets, or isopropyl (J = 5 Hz - a little small)

6 B δ 1.27, 3H, t, J = 7Hz CH_3-CH_2-

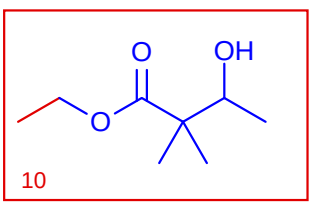
C δ 2.70, 1H, t, J = 7 Hz -O-H

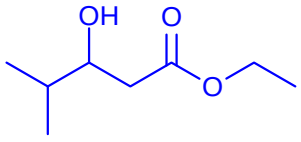
D δ 3.86, 1H, pentet, J = 7 Hz CH_3-C(H)-OH

E δ 4.17, 2H, q, J = 7 Hz $-O-CH_2-CH_3$

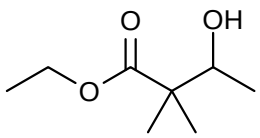
(f) Give your answer below. If more than one structure fits the data, draw them, but indicate your best choice by circling the structure

10





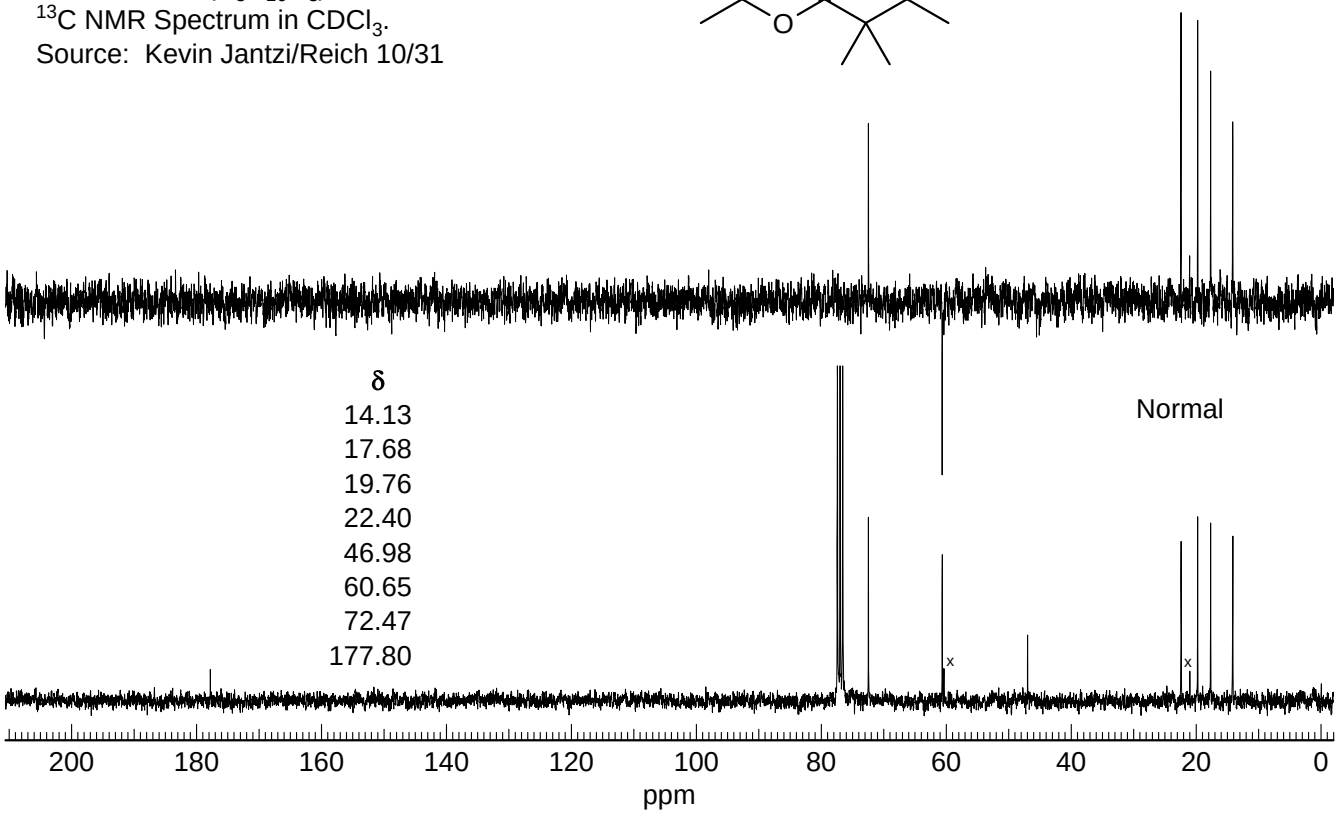
Problem R-10E ($C_8H_{16}O_3$).
^{13}C NMR Spectrum in $CDCl_3$.
Source: Kevin Jantzi/Reich 10/31



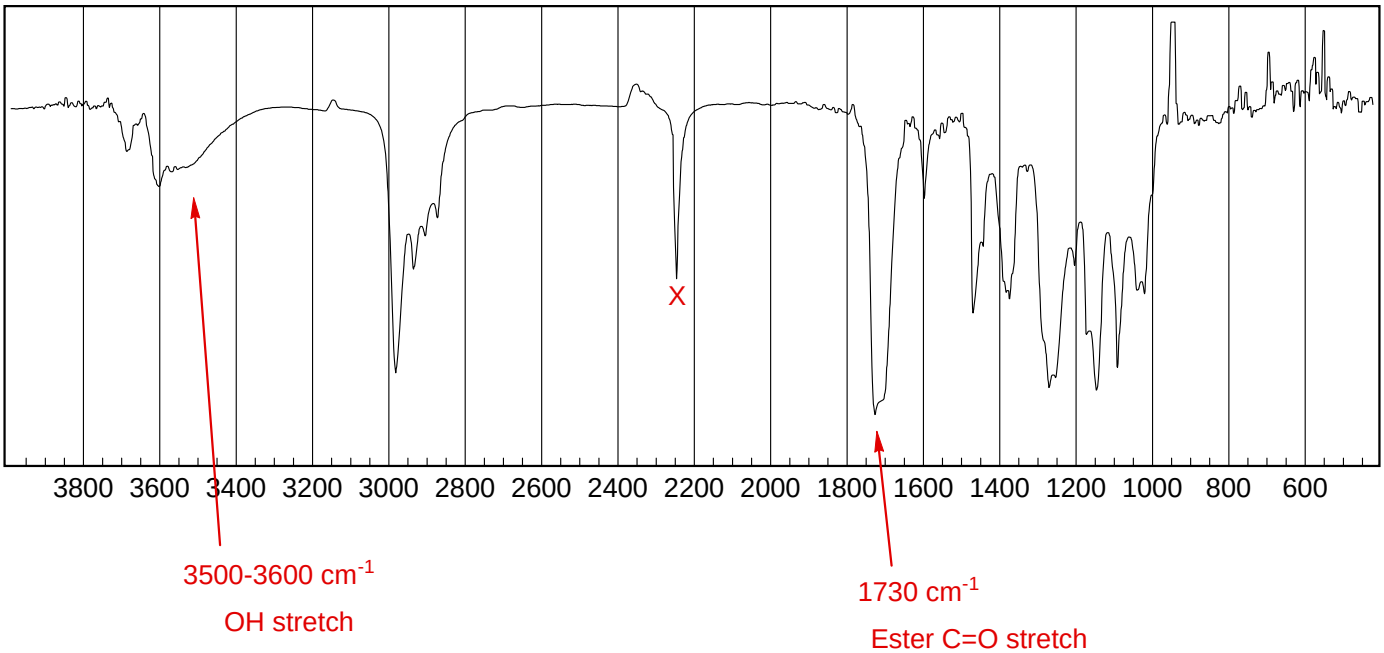
DEPT 135

δ
14.13
17.68
19.76
22.40
46.98
60.65
72.47
177.80

Normal



Problem R-10E ($C_8H_{16}O_3$).
IR Spectrum Neat
Source: Nicolet FT-IR



PLT ex-1-2010-11-gq.plt