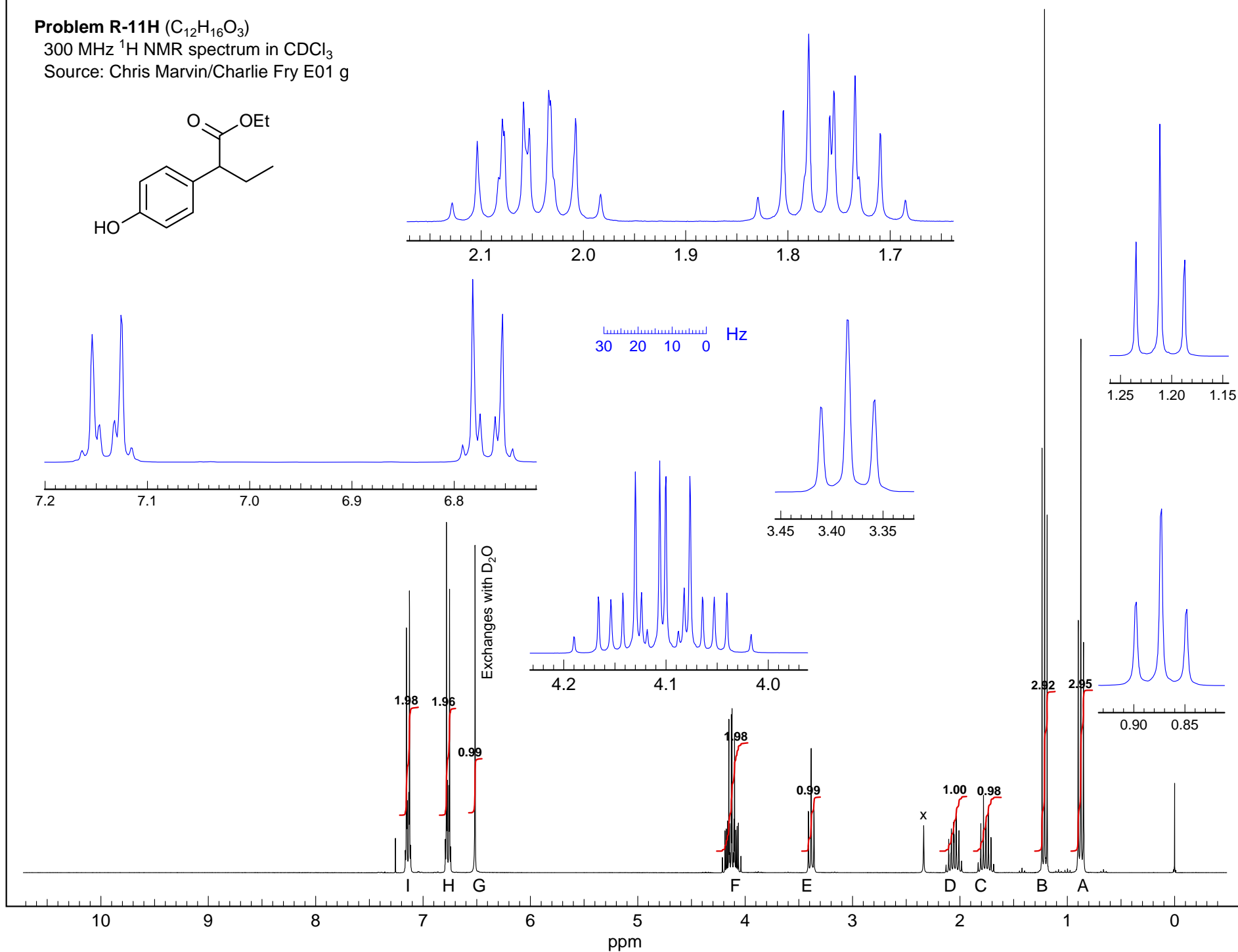
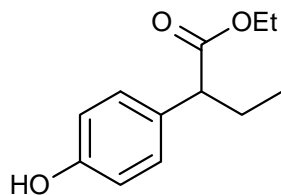


Problem R-11H (C₁₂H₁₆O₃)

300 MHz ¹H NMR spectrum in CDCl₃

Source: Chris Marvin/Charlie Fry E01 g

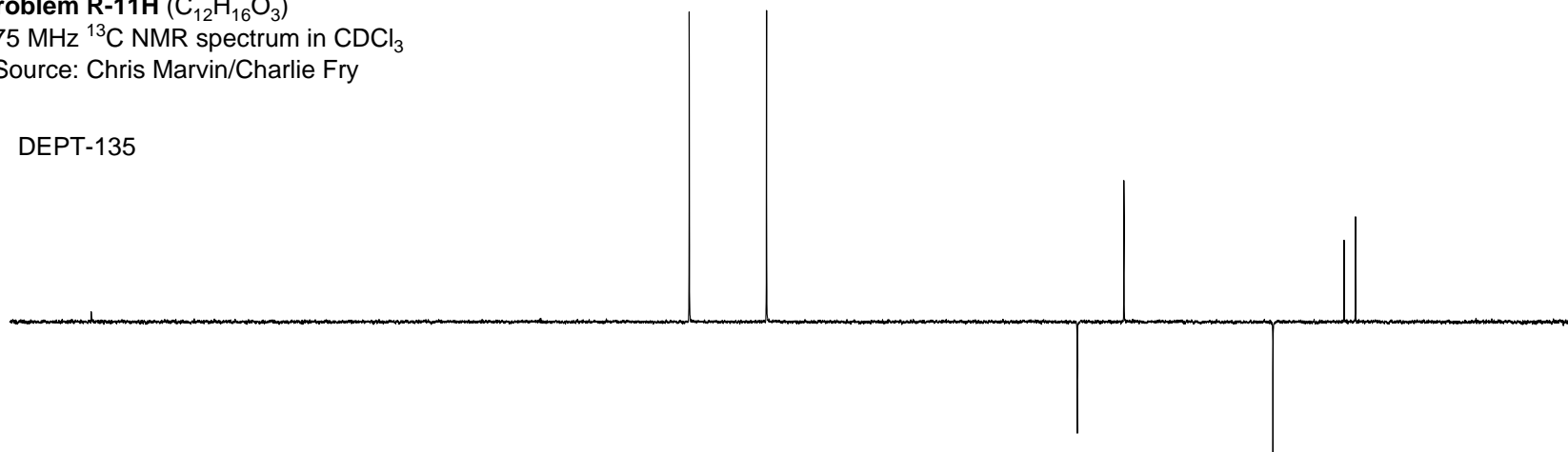


Problem R-11H (C₁₂H₁₆O₃)

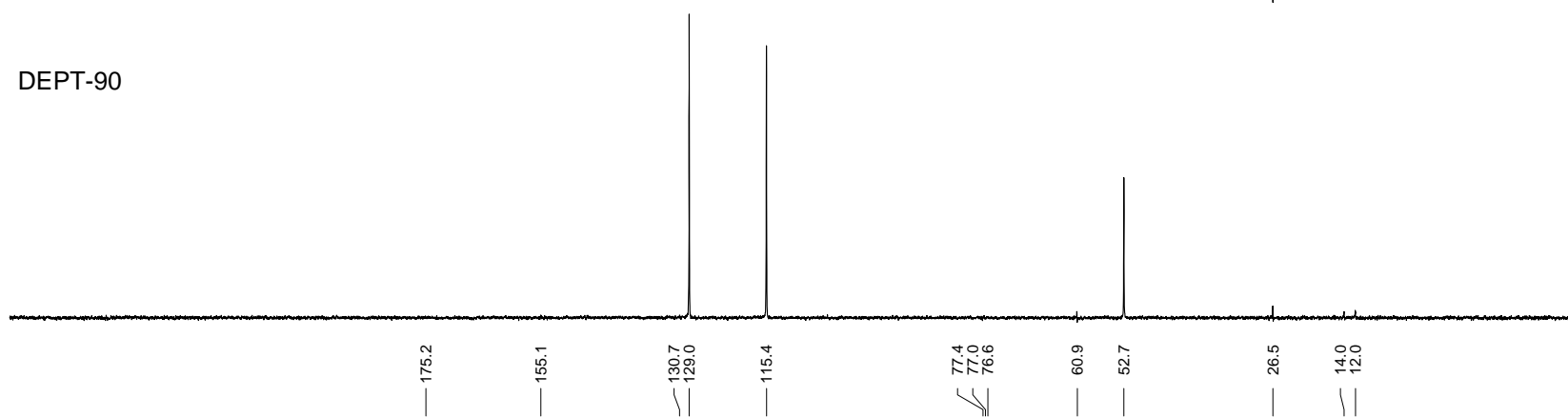
75 MHz ¹³C NMR spectrum in CDCl₃

Source: Chris Marvin/Charlie Fry

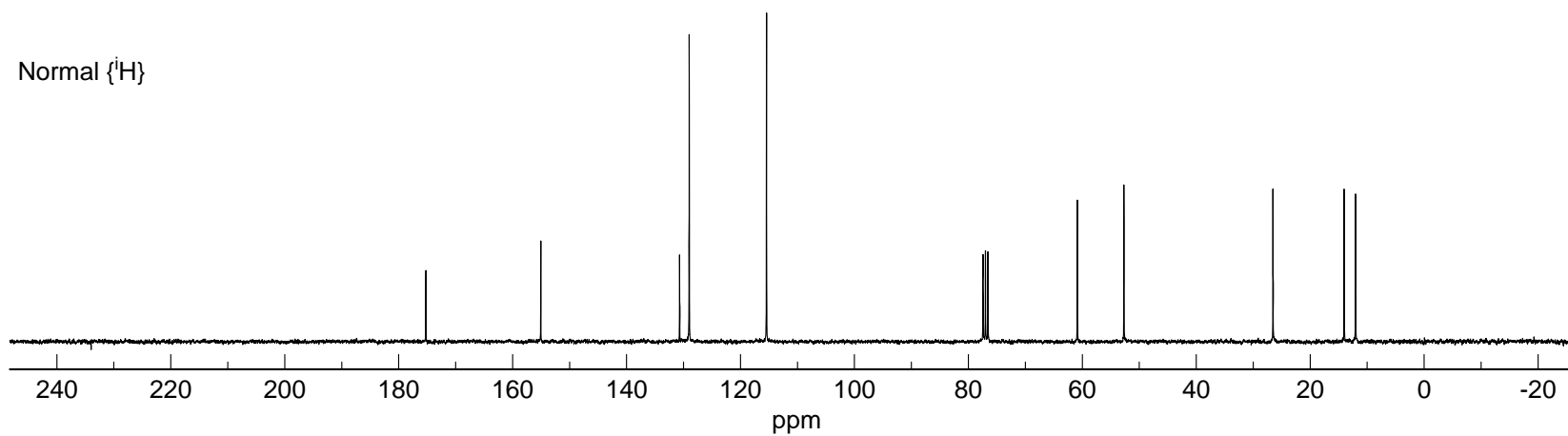
DEPT-135



DEPT-90



Normal {¹H}

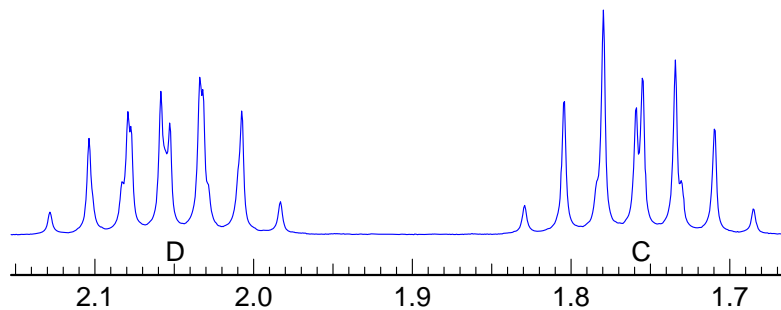


Problem R-11H ($C_{12}H_{16}O_3$). You are provided the 1H and ^{13}C NMR spectra of a compound. Interpret the spectra, and determine the structure or structures. Note that the signal at δ 6.5 disappeared when D_2O was added.

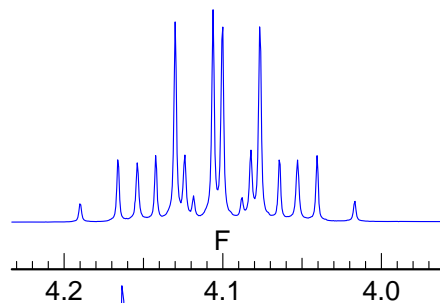
(a) DBE _____

(b) Analyze the multiplets below. Identify the patterns (e.g., ABXYZ - underline the observed nuclei). If they are first order, report them in the standard format (δ 0.00, dqt, $J = 0.0, 0.0, 0.0, 2H$). Provide part structure(s) defined by these protons.

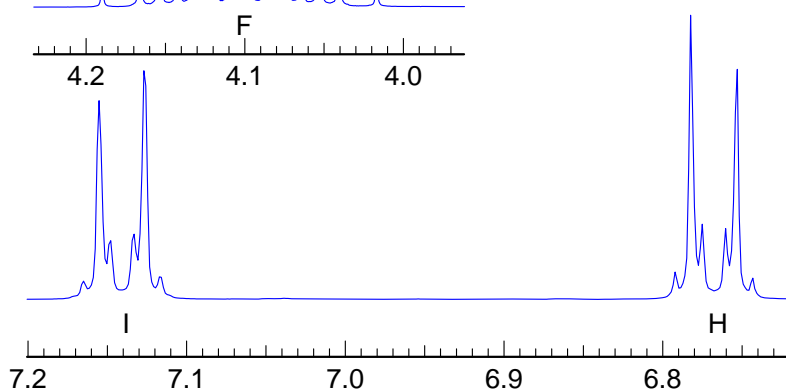
δ 1.7-2.1 _____



δ 3.9-4.1 _____



δ 6.7-7.2 _____



(c) Identify at least 3 signals in the ^{13}C NMR spectrum which provide significant structural information, and describe the part structures obtained from them.

(d) Draw the structure of **R-11H** below. If more than one structure fits the data, draw them, but circle your best choice.

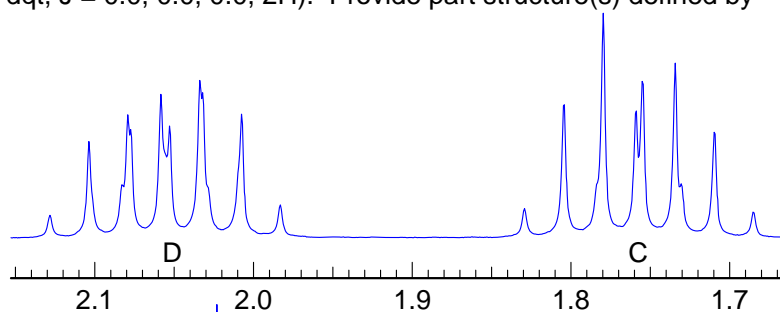
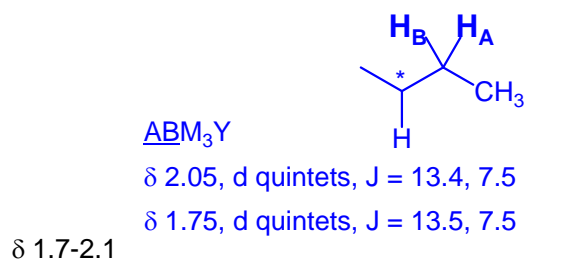
30

Problem R-11H ($C_{12}H_{16}O_3$). You are provided the 1H and ^{13}C NMR spectra of a compound. Interpret the spectra, and determine the structure or structures. Note that the signal at δ 6.5 disappeared when D_2O was added.

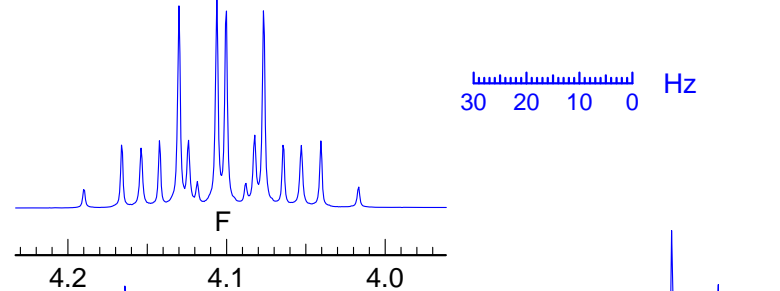
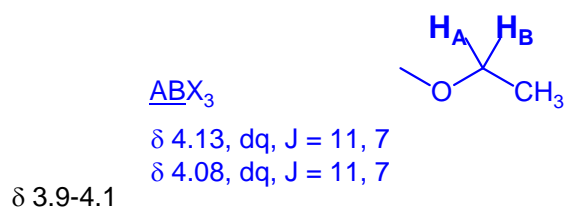
2 (a) DBE 5

(b) Analyze the multiplets below. Identify the patterns (e.g., ABXYZ - underline the observed nuclei). If they are first order, report them in the standard format (δ 0.00, dqt, $J = 0.0, 0.0, 0.0, 2H$). Provide part structure(s) defined by these protons.

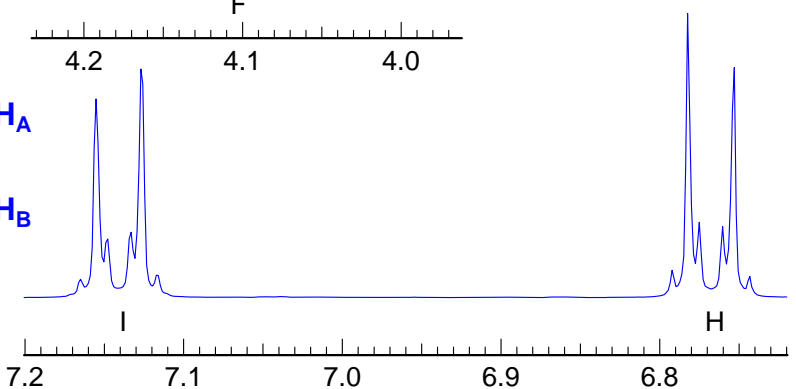
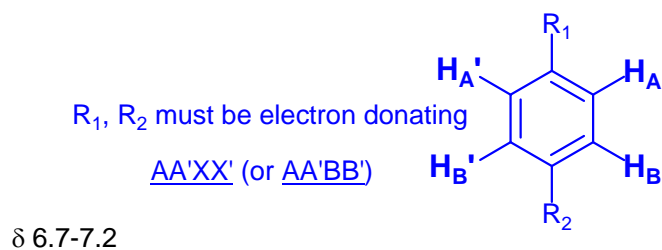
5



5



5



(c) Identify at least 3 signals in the ^{13}C NMR spectrum which provide significant structural information, and describe the part structures obtained from them.

δ 175.2 - This is an ester carbonyl carbon

δ 155.1 - This is likely an sp^2 carbon (aromatic) bearing an electronegative group C-O

3

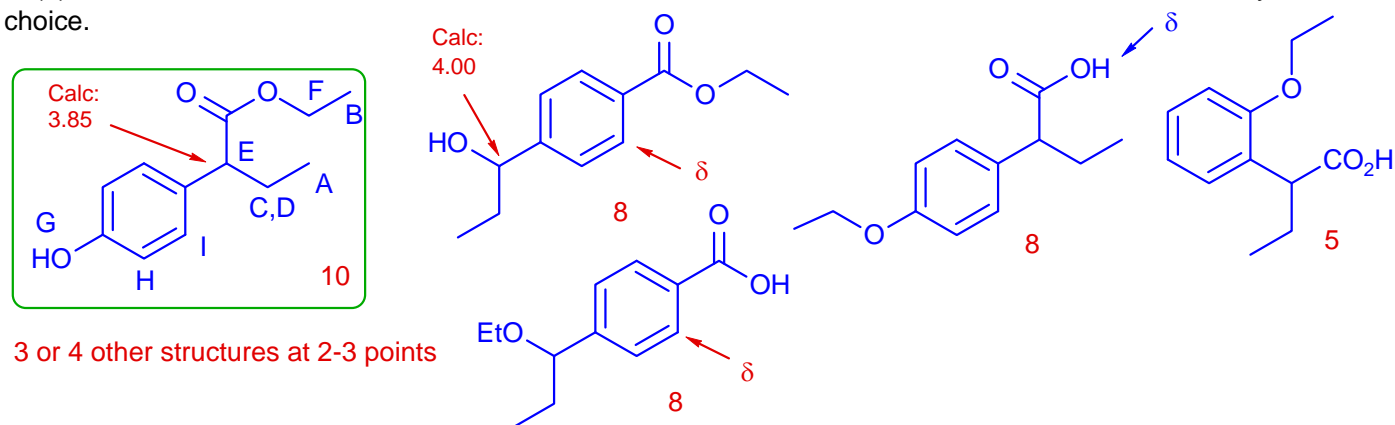
δ 60.9 - sp^3 carbon, probably a CH_2 -O group

δ 52.7 - sp^3 CH

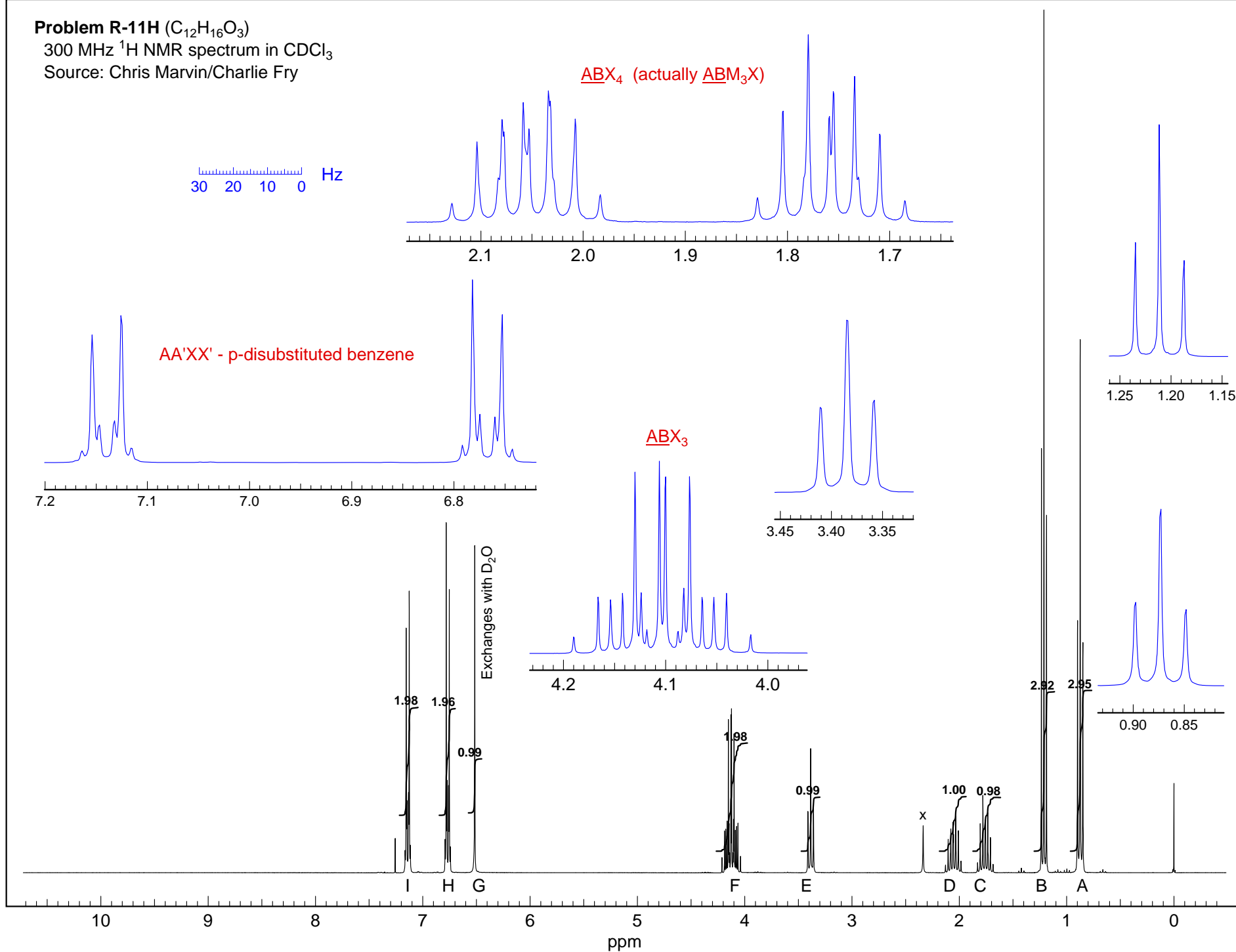
There are also two CH_3 carbons (neither one on O) and an aliphatic CH (52.7), also probably not on O

(d) Draw the structure of **R-11H** below. If more than one structure fits the data, draw them, but circle your best choice.

10



Problem R-11H ($C_{12}H_{16}O_3$)
 300 MHz 1H NMR spectrum in $CDCl_3$
 Source: Chris Marvin/Charlie Fry

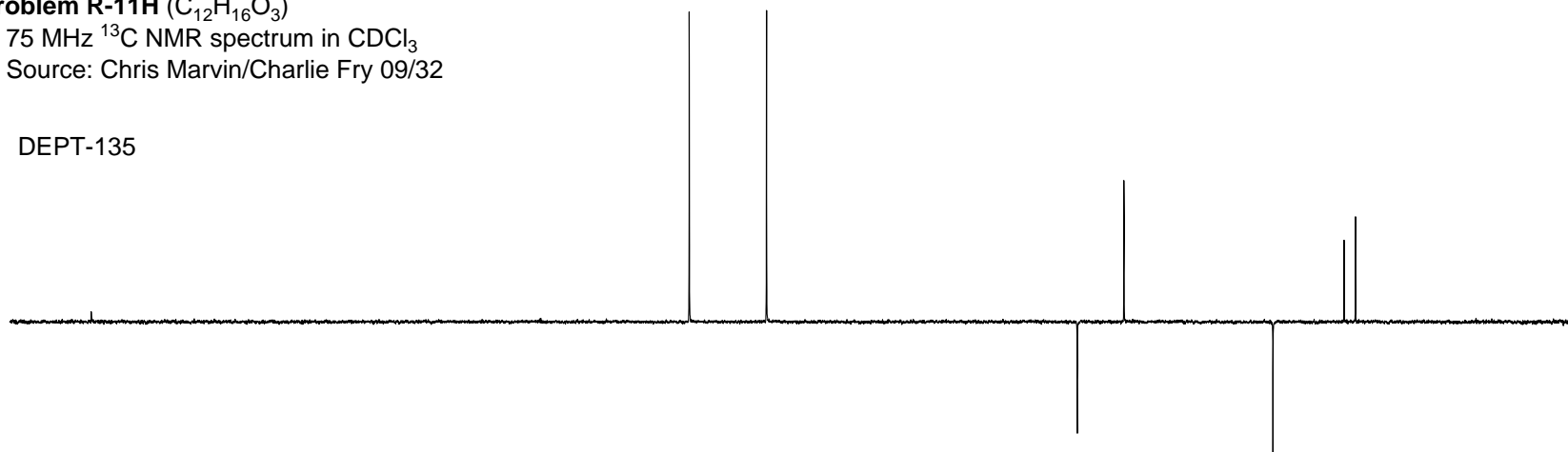


Problem R-11H (C₁₂H₁₆O₃)

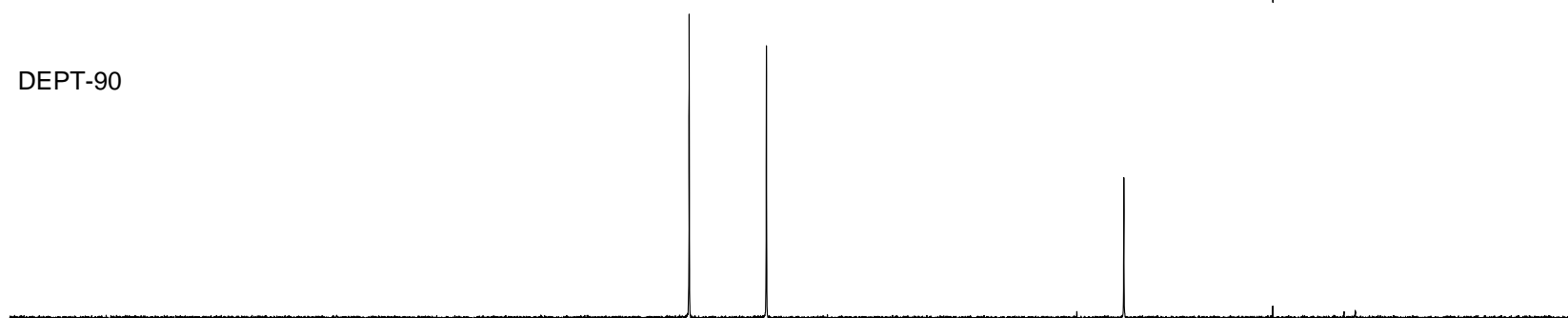
75 MHz ¹³C NMR spectrum in CDCl₃

Source: Chris Marvin/Charlie Fry 09/32

DEPT-135



DEPT-90



Normal {¹H}

