

Practice Exam 2

Chemistry 605 (Reich)

SECOND HOUR EXAM

Thur. April 14, 2011

Question/Points

R-10F _____/25

R-10G _____/20

R-10H _____/10

R-10I _____/25

R-10J _____/20

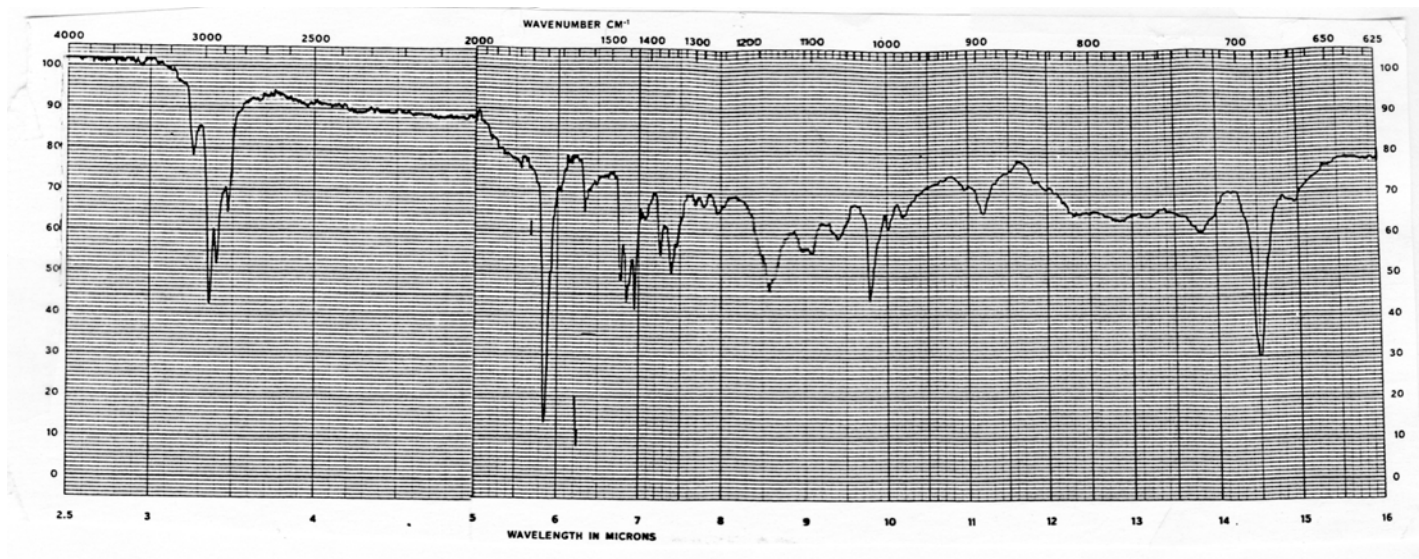
Total _____/100

Name _____

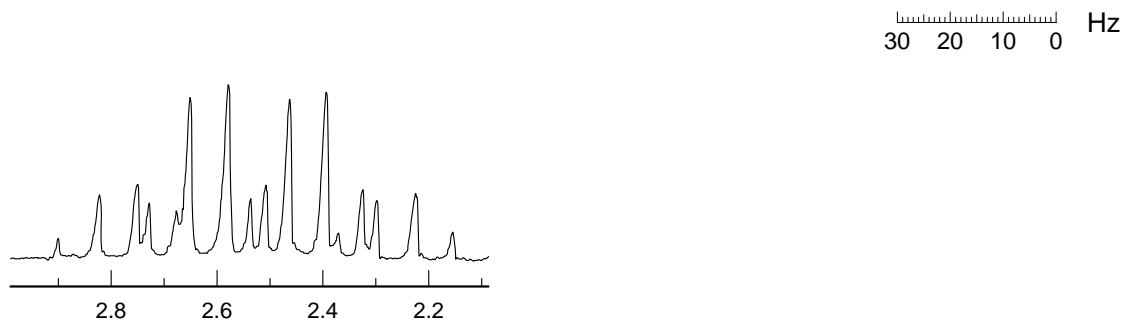
If you place answers anywhere else except in the spaces provided, (e.g. on the spectra or on extra pages) clearly indicate this on the answer sheets.

Problem R-10F ($C_{12}H_{16}OSe$). In this problem you are required to determine a structure from the IR and 1H NMR spectra of a compound. The compound contains a Ph-Se group.

(a) DBE _____. (b) Report your analysis of the IR spectrum (CCl_4). List the data and any conclusions you drew from it.



(c) Interpret the 2-proton multiplet at δ 2 to δ 3. What do these signals tell you about the structure. Draw a coupling tree above it to show you understand the multiplet.



(c) Interpret the remaining multiplets in the NMR spectrum. Give multiplicity, coupling constants and part structures you were able to obtain from the signal.

δ 1.0 _____

δ 1.7 _____

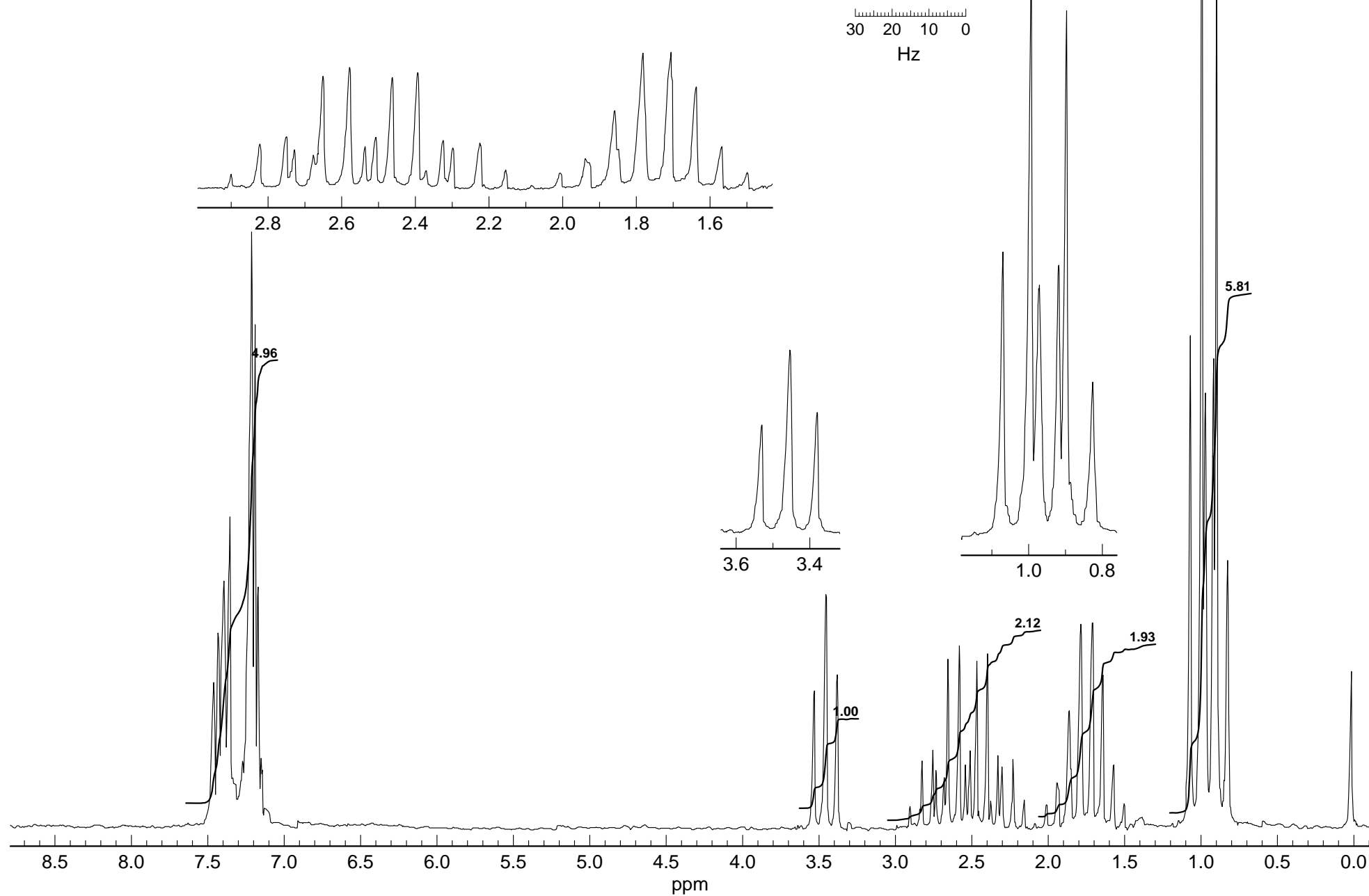
δ 3.5 _____

e) Draw the structure of R-10F below. Label it with chemical shifts.

Problem R-10F ($\text{C}_{12}\text{H}_{16}\text{OSe}$)

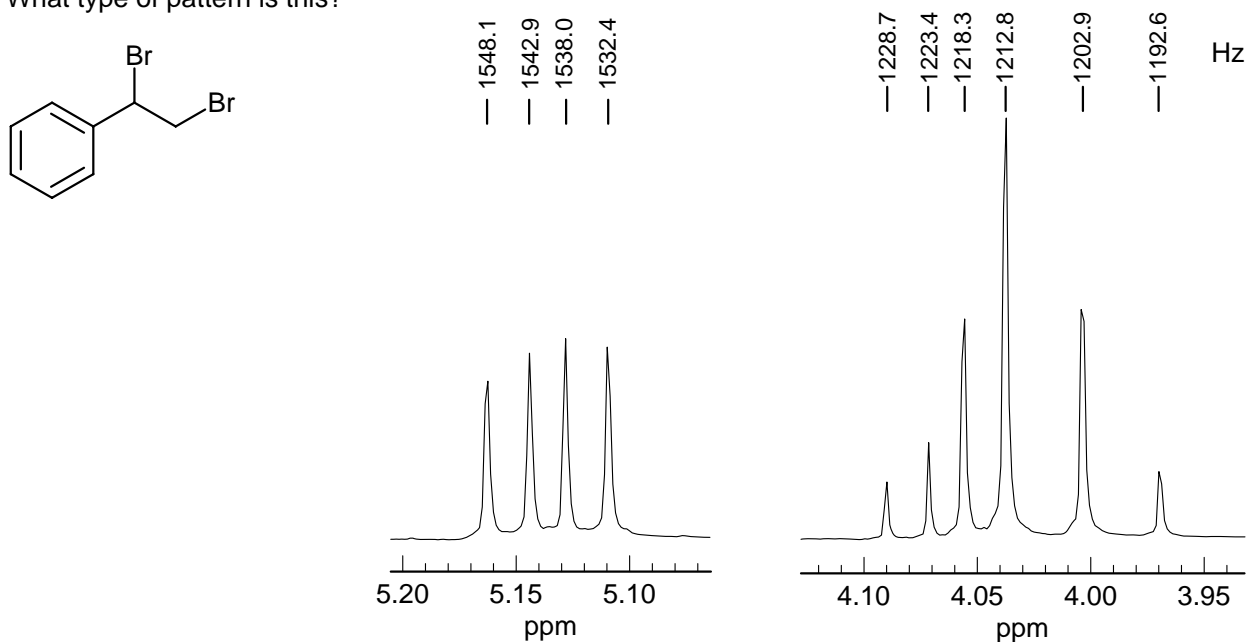
100 MHz ^1H NMR Spectrum in CCl_4

(Source: Hans Reich 12/18)

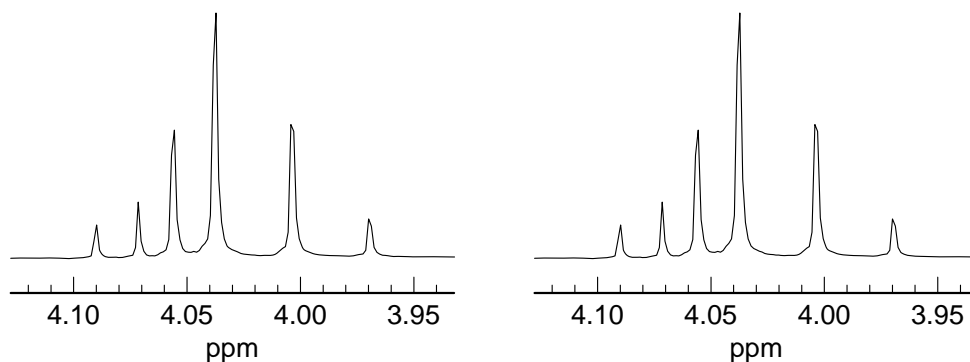


Problem **R-10G** ($C_8H_8Br_2$). This problem requires you to analyze the signals at δ 4.1 and δ 5.2. You are given the structure.

(a) Do a "first order" analysis of the two multiplets shown below. Draw a coupling tree, and estimate couplings. What type of pattern is this?



(b) Do an accurate (quantitative) analysis. Use the frequencies shown above. If more than one solution is possible, show them both, and draw the proper coupling tree on the spectra below. Use appropriate criteria to distinguish the two. Show your work, and tabulate your data in an easily readable form.

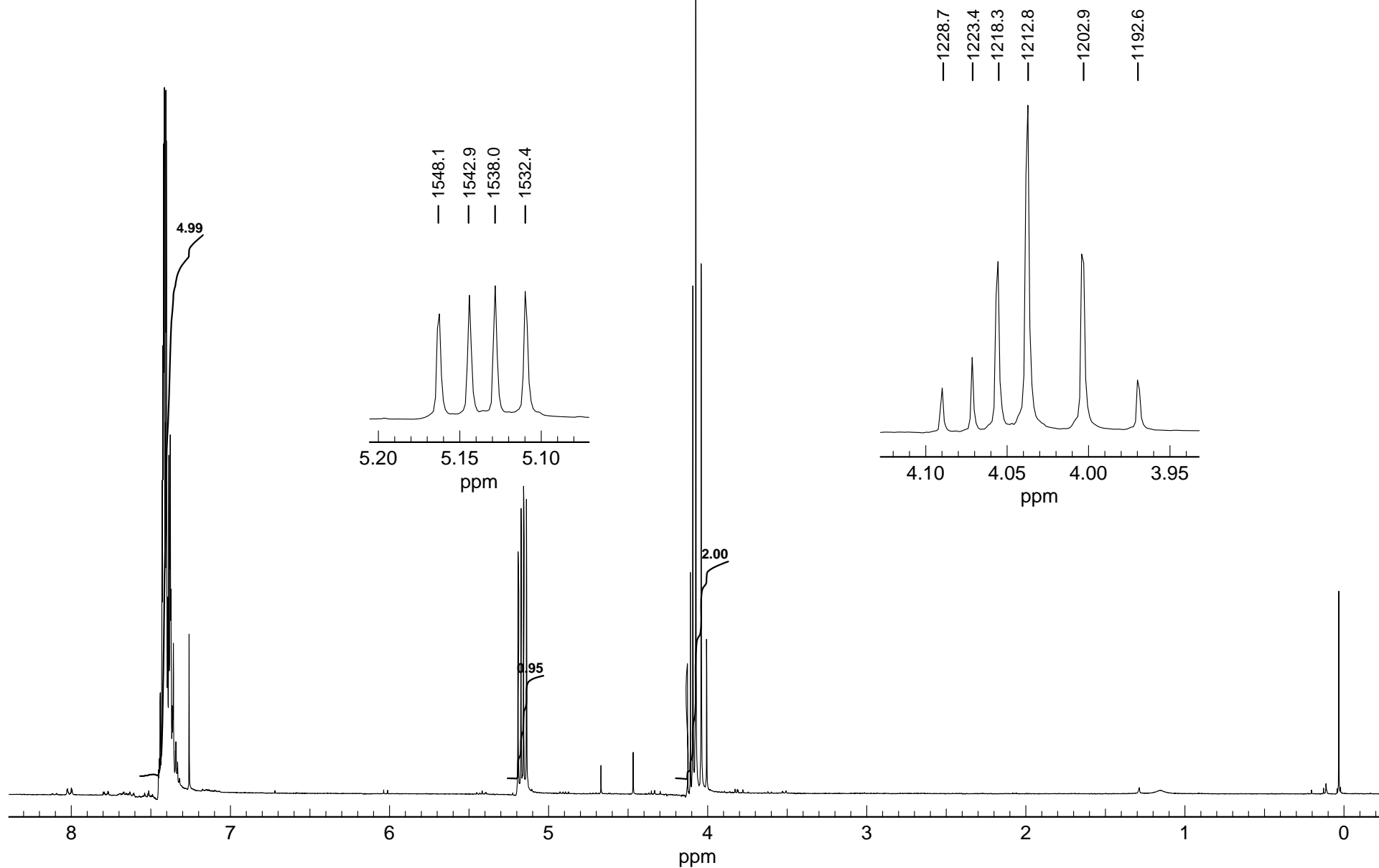


Problem R-10G ($\text{C}_8\text{H}_8\text{Br}_2$)

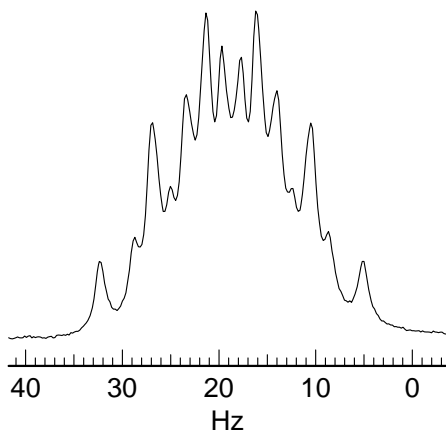
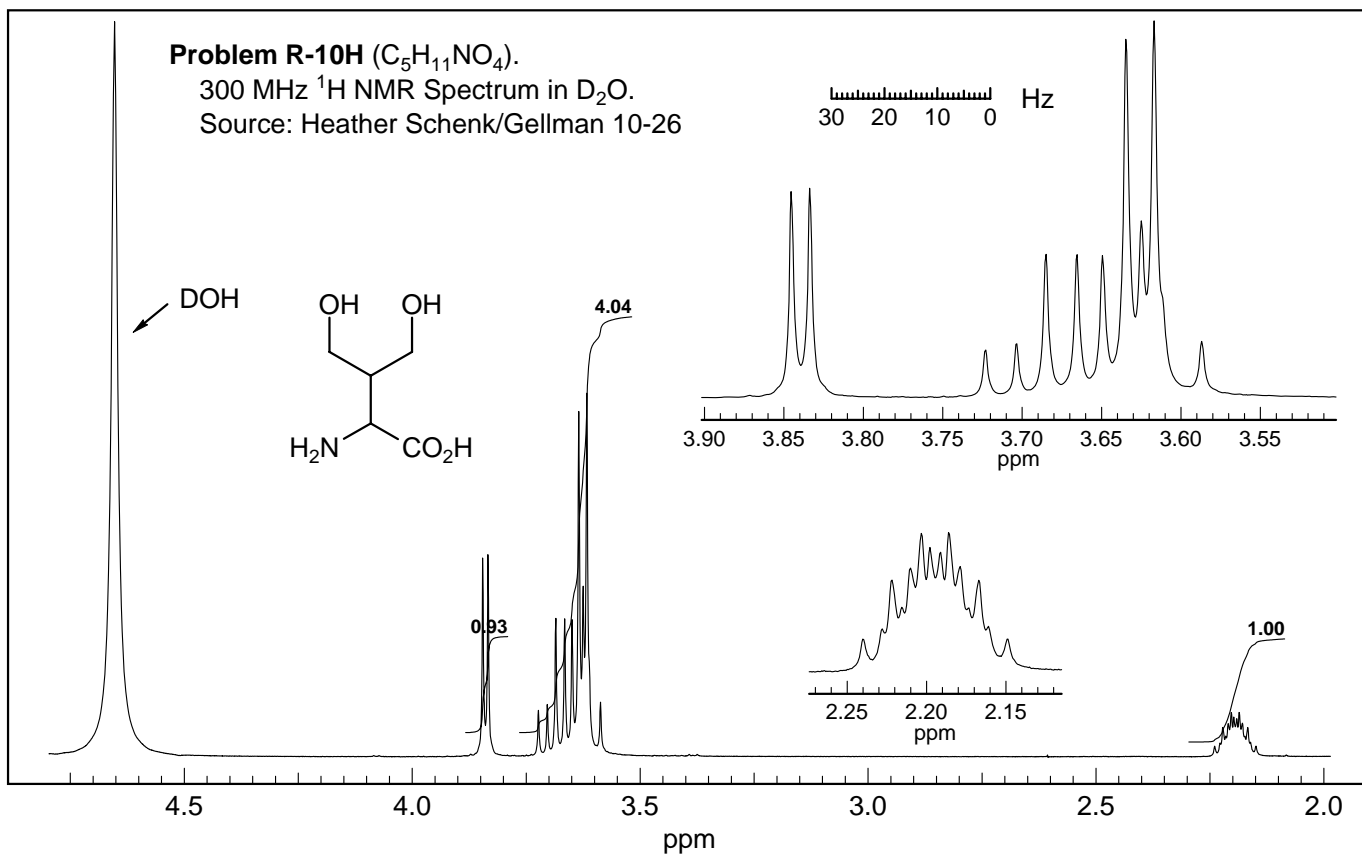
300 MHz ^1H NMR Spectrum in CDCl_3

(Source: Wayne Goldenberg/Reich 11/31)

30 20 10 0
Hz



Problem R-10H ($C_5H_{11}NO_4$). A graduate student thought she had prepared the compound below, but was worried about the NMR spectrum (taken in D_2O), which seemed more than a little odd. Does the NMR spectrum fit the structure? Analyze and assign each of the multiplets. In particular, provide an explanation for the appearance of the key multiplet δ 3.5-3.8.



To show you understand the spectrum, draw a coupling tree for the multiplet at δ 2.2 (start with an intensity assignment).

Problem R-10I ($C_{12}H_8Cl_4$). You are provided the 1H NMR spectrum of a compound. Interpret the NMR spectrum, and determine the structure or structures. Use the A, B, etc labels on the spectrum. Show the chemical shift and multiplet structure in the form: 0.0 δ , dtd, $J_{AB} = 0.0, 0.0, 0.0$ Hz, 1H . You may use first order analysis.

(a) DBE _____

(b) Analyze the multiplets A, B, C. Provide part structure(s) defined by these protons. **Note: Do not attempt to distinguish among the several isomers which are consistent with this pattern.**

A _____

B _____

C _____

(c) Interpret the signals D-H. Provide part structure(s) defined by these protons.

D _____

E _____

F _____

G _____

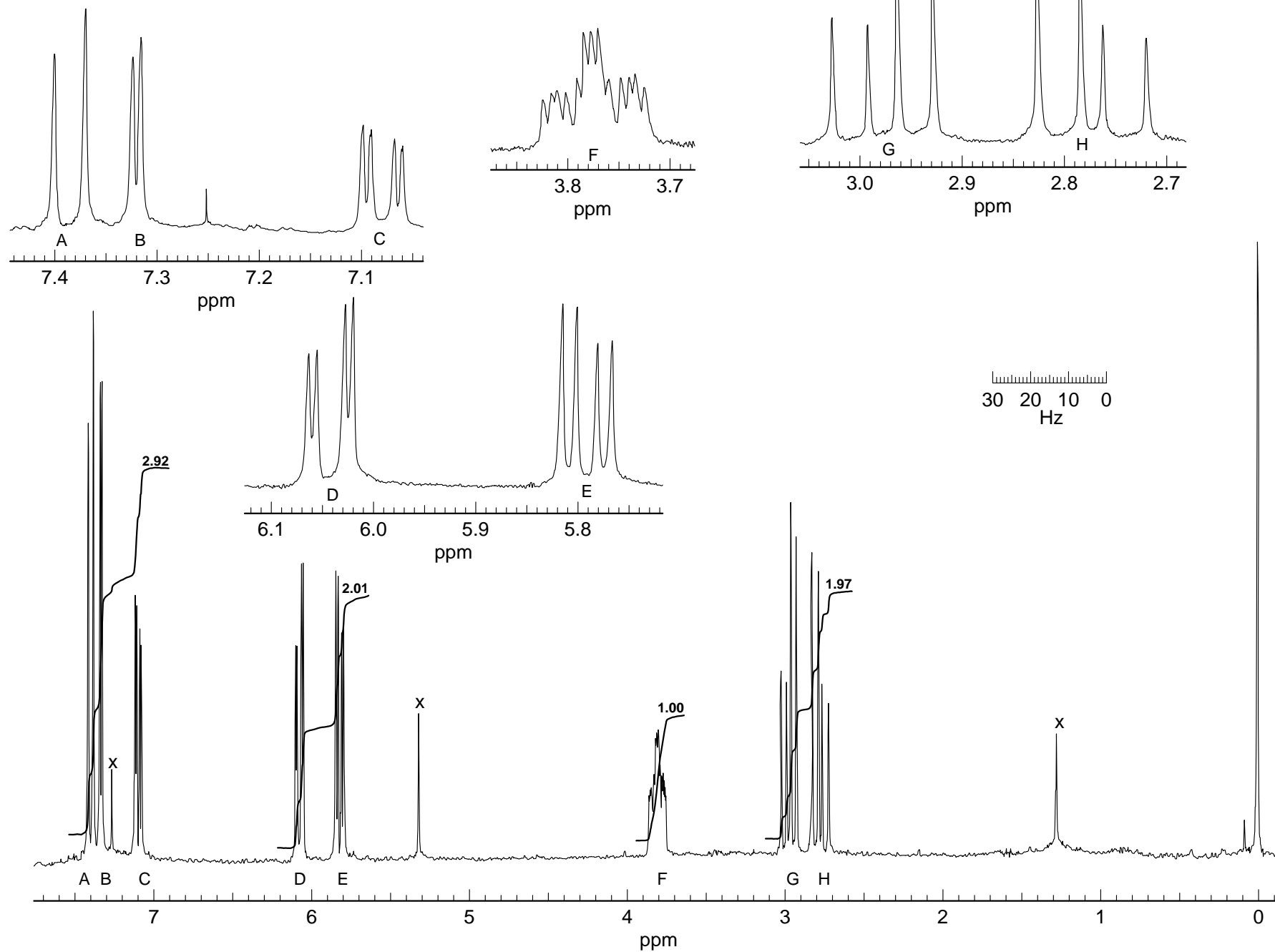
H _____

(d) Draw the structure of **R-00F** below. If more than one structure fits the data, draw them, but circle your first choice. Assign the protons (label them with the letters A-H). If any assignments are ambiguous, indicate the basis for your choice.

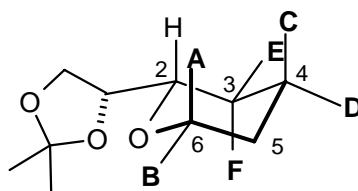
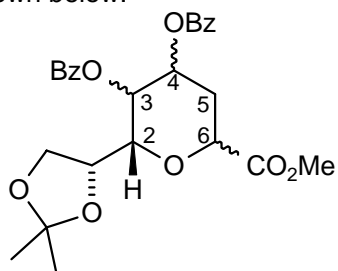
Problem R-10I ($C_{12}H_8Cl_4$).

270 MHz 1H NMR Spectrum in $CDCl_3$.

Source: Ieva Reich 10/30



Problem R10J ($C_{24}H_{28}O_9$). This problem requires you to analyze part of the 1H NMR spectrum of a tetrahydropyran, and determine the stereochemistry at three centers. A planar projection and conformational drawing is shown below.



Bz = $PhC(=O)-$

(a) Determine the stereochemistry at C-6. Explain what signal(s) you used, give their shift and multiplicity (e.g. δ 0.00, tq, $J=0$, 0) and briefly describe how you made the stereochemical assignment using the data:

A = _____, B = _____ (H or CO_2Me).

(b) Determine the stereochemistry at C-4. Explain what signal(s) you used, give their shift and multiplicity and briefly describe how you made the stereochemical assignment using the data:

C = _____, D = _____ (H or OBz).

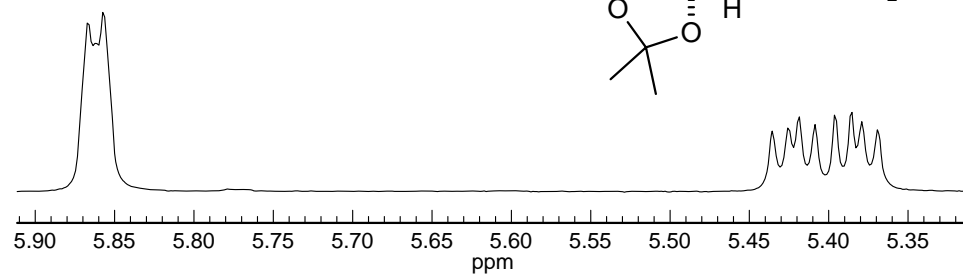
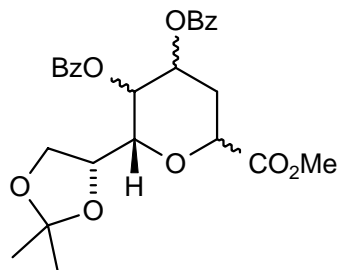
(c) Determine the stereochemistry at C-3. Explain what signal(s) you used, give their shift and multiplicity and briefly describe how you made the stereochemical assignment using the data:

E = _____, F = _____ (H or OBz).

Problem R-10J (C₂₄ H₂₈ O₉)

300 MHz ¹³C NMR Spectrum in CDCl₃

Source: Geoffrey Sametz/Burke 9/99



30 20 10 0 Hz

