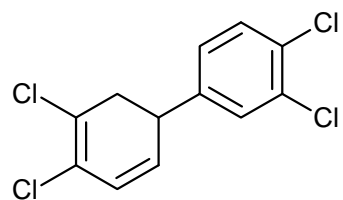


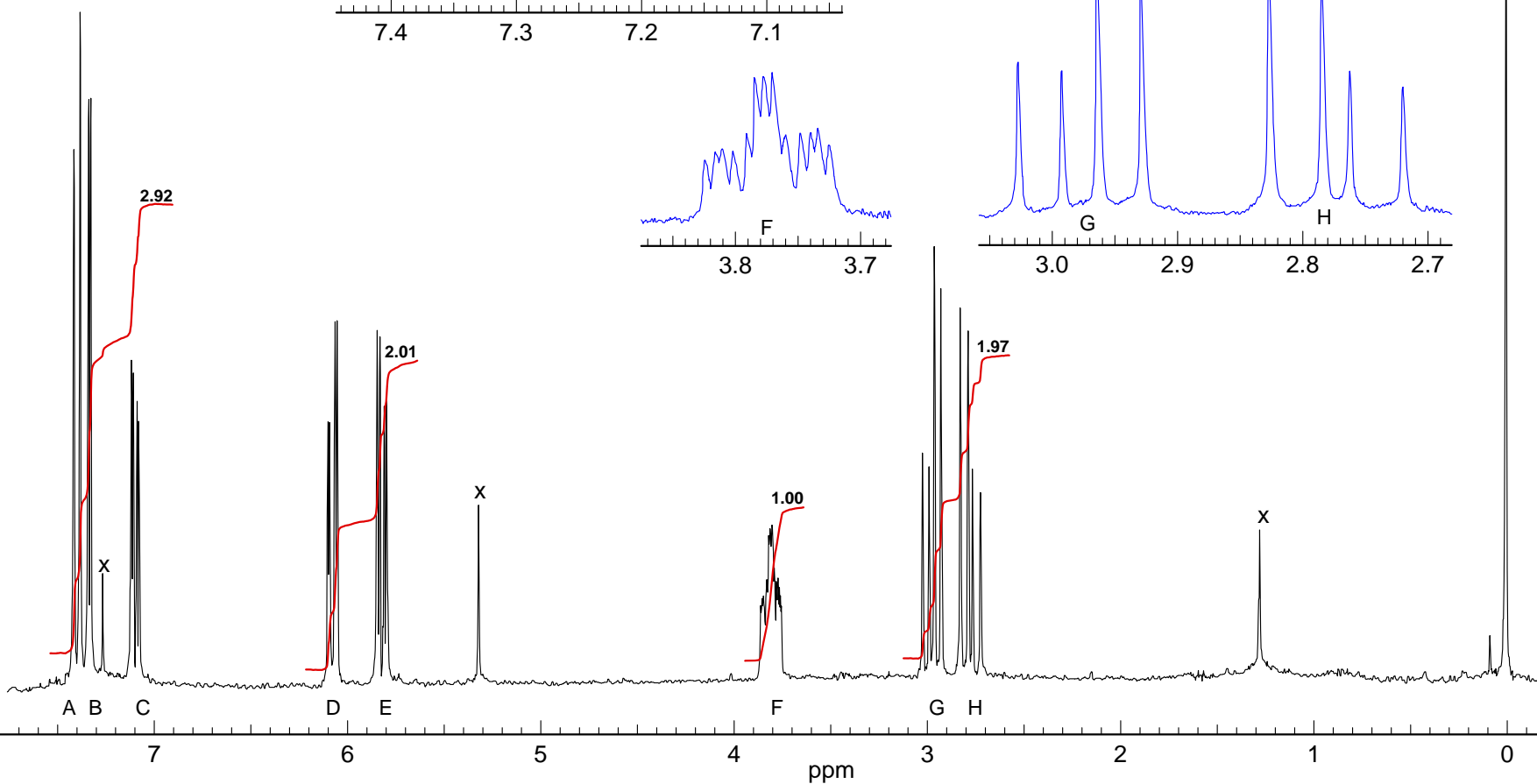
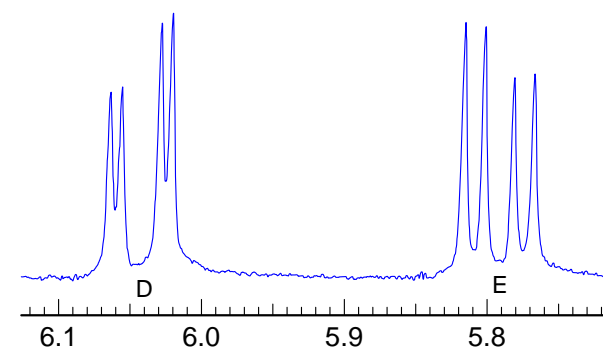
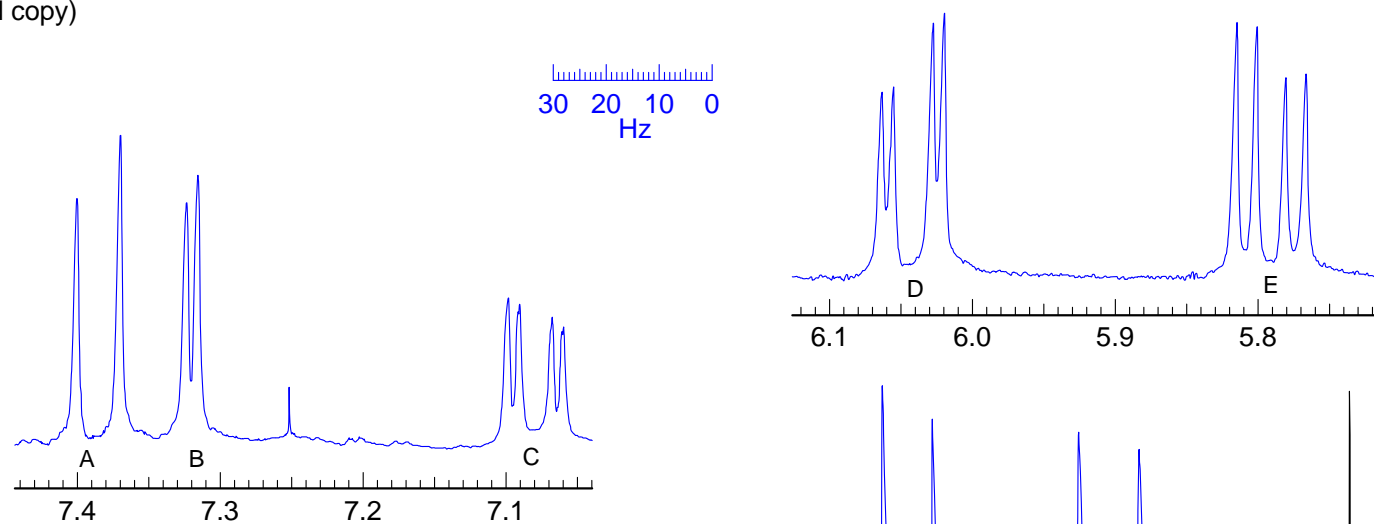
Problem R-10I ($C_{12}H_8Cl_4$).

270 MHz 1H NMR Spectrum in $CDCl_3$.

Source: Ieva Reich (digitized hard copy)



30 20 10 0
Hz



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-101 ($C_{12}H_8Cl_4$). 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.

2

(a) DBE 7

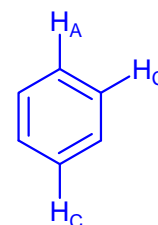
(b) Analyze the multiplets A, B, C. Provide part structure(s) defined by these protons. **Note: Do not attempt to distinguish among the several isomers which are consistent with this pattern.**

A δ 7.39, d, $J = 8$ Hz (J-ortho)

B δ 7.32, d, $J = 2$ Hz (J-meta)

C δ 7.08, dd, $J = 8, 2$ Hz (J-ortho + J-meta)

These are aromatic protons and define a 1,2,4-trisubstituted benzene



5

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

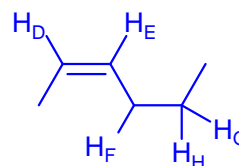
D δ 6.04, dd, $J = 9, 2$ Hz

E δ 5.79, dd, $J = 10, 4$ Hz

F δ 3.78, dddd, $J = 11, 10, 4, 2$ Hz

G δ 2.97, dd, $J = 17, 9.5$ Hz

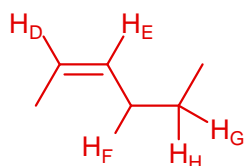
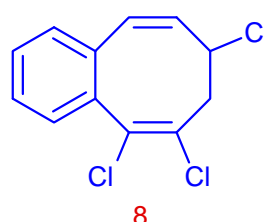
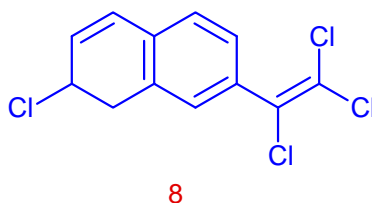
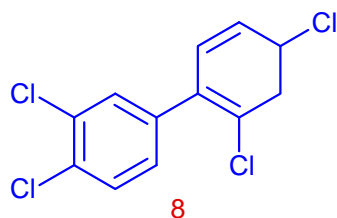
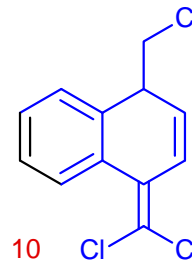
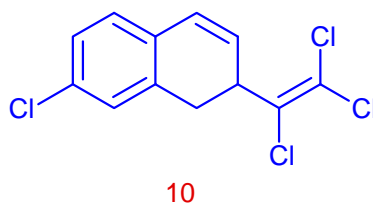
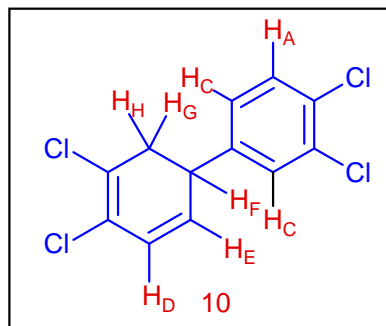
H δ 2.78, dd, $J = 17, 11$ Hz



8

(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.

10



This question elicited many answers - not a good problem since there are too many hidden carbons.

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

270 MHz 1H NMR Spectrum in $CDCl_3$.

Source: Ieva Reich (digitized hard copy)

