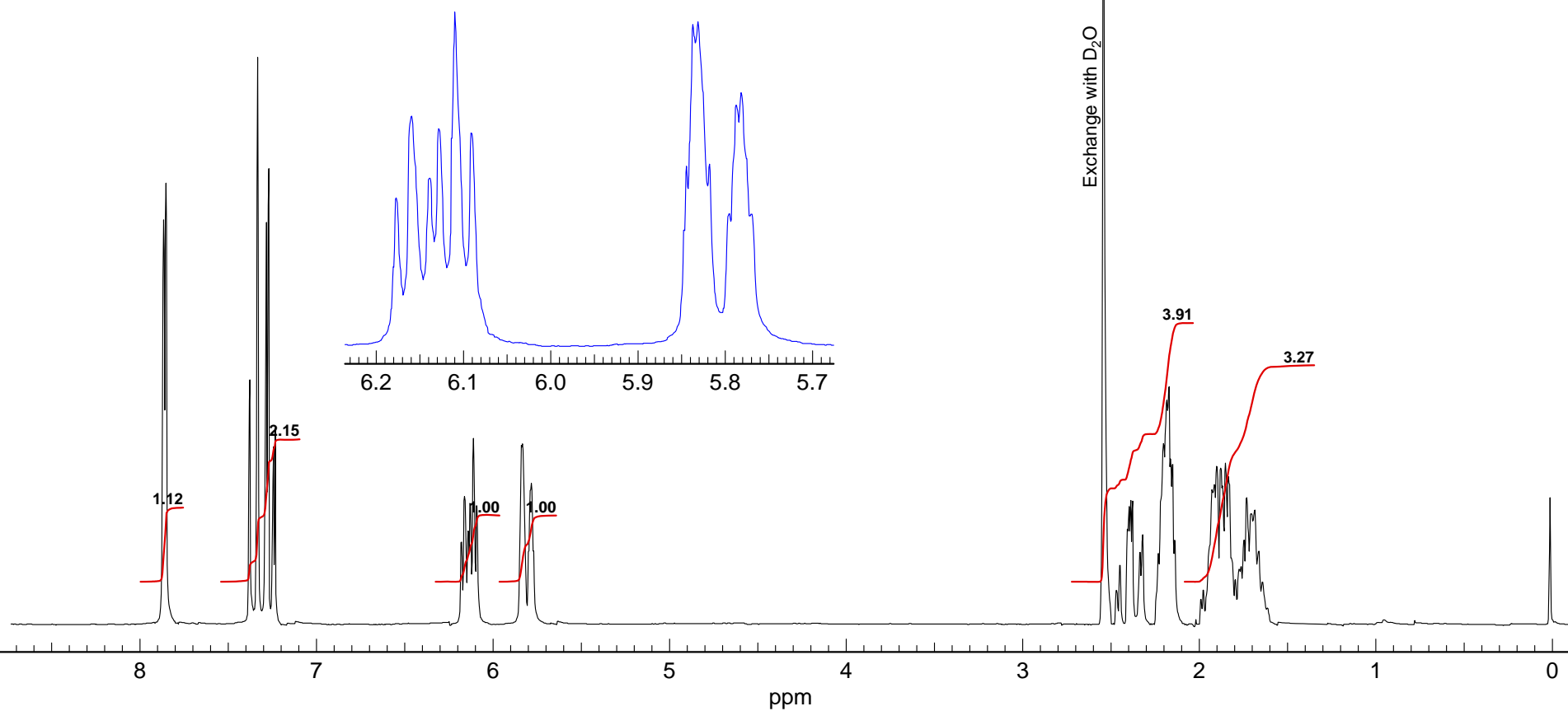
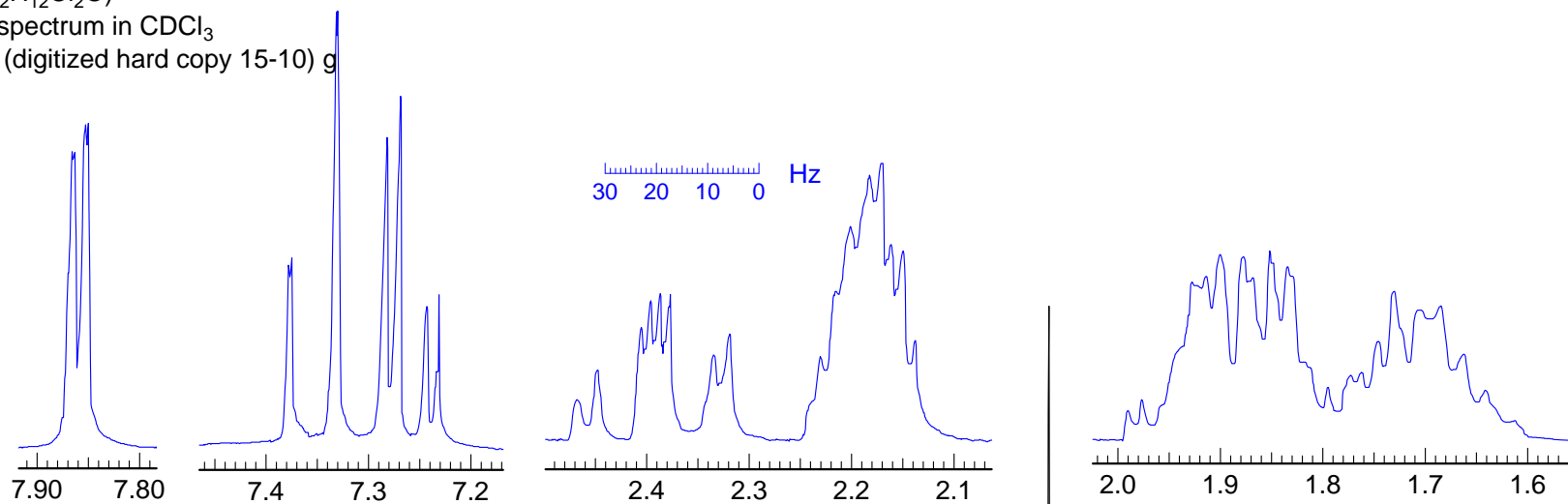
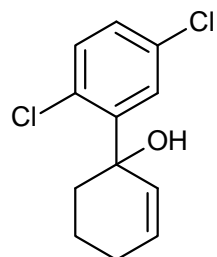


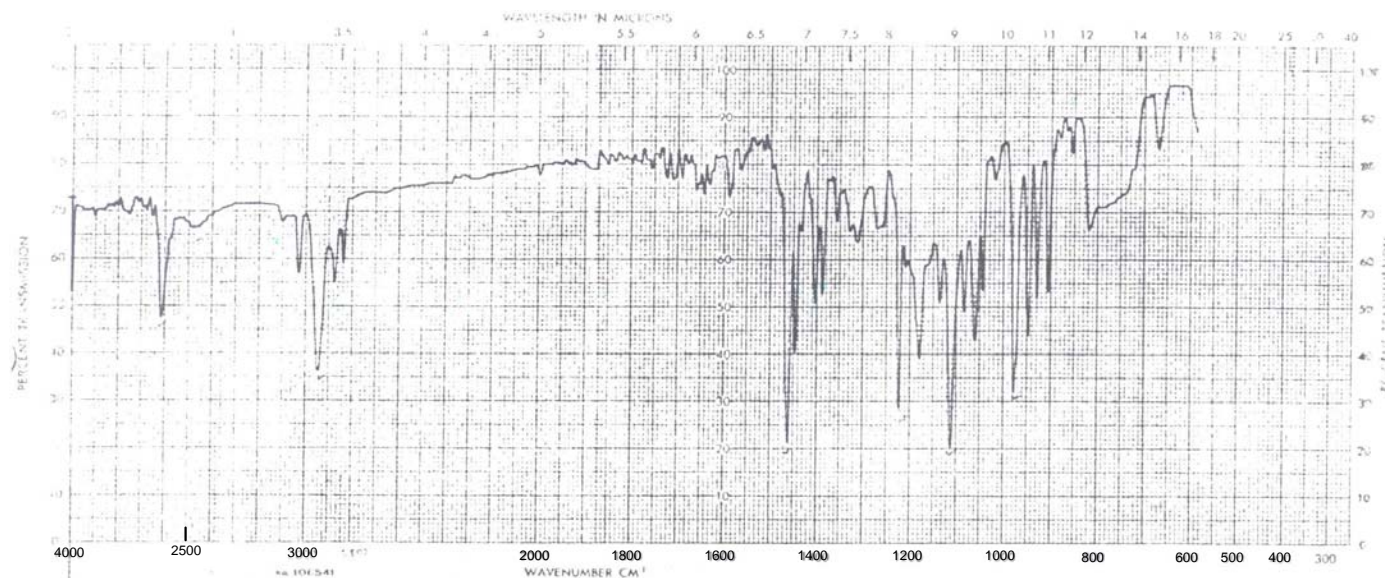
Problem R-85A ($C_{12}H_{12}Cl_2O$)

200 MHz 1H NMR spectrum in $CDCl_3$

Source: I. L. Reich (digitized hard copy 15-10) g



Problem R-85A ($C_{12}H_{12}Cl_2O$) Determine the structure from the 200 MHz NMR spectrum and the IR spectrum



(a) DBE ____ Interpret the IR spectrum.

(b) What do you conclude from the NMR signals at δ 7 to δ 8? Draw a part structure, label with δ and J values.

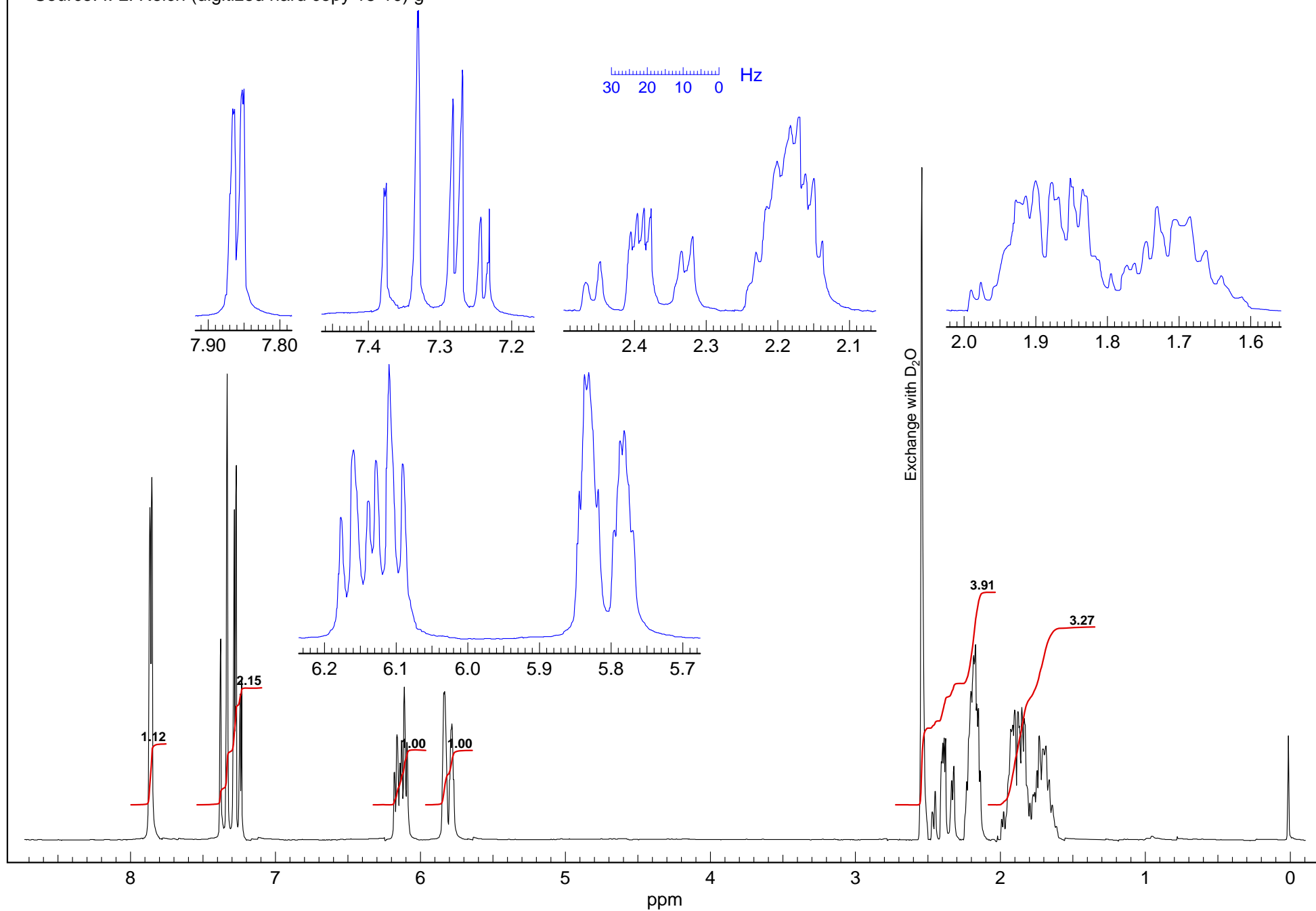
(c) What do you conclude from the NMR signals at δ 5.5 to 6.5? Draw a part structure and label with δ and J values.

(d) Assign a structure or partial structure to R-85A and identify any structural features you could not establish firmly.

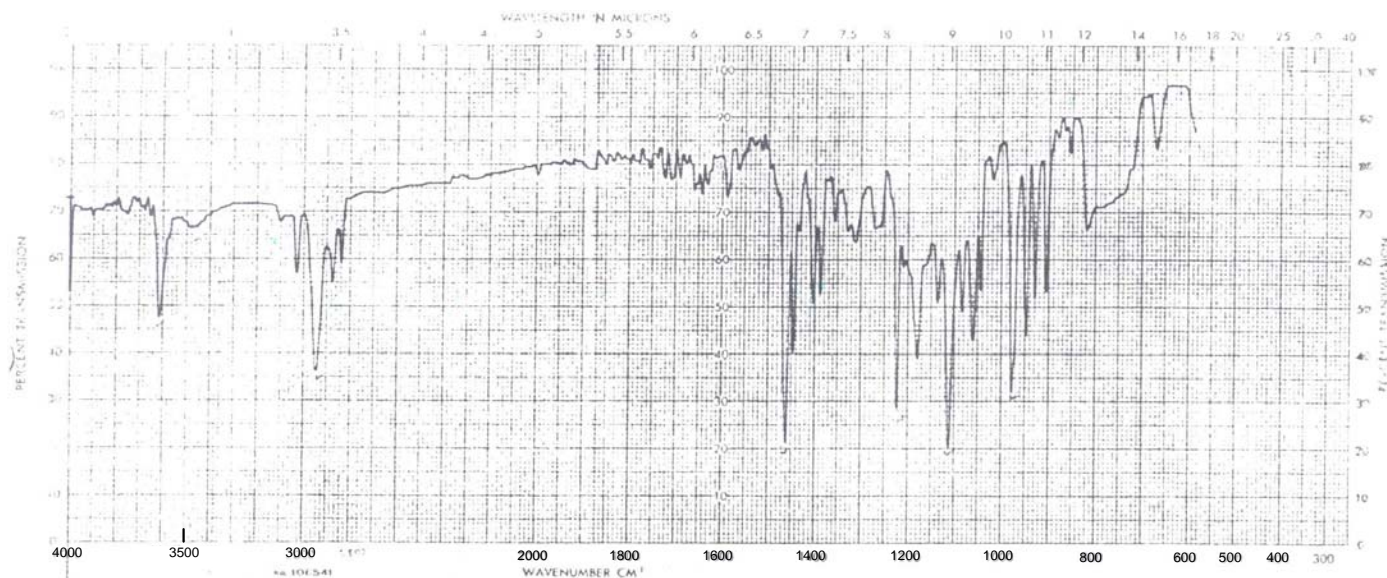
Problem R-85A ($C_{12}H_{12}Cl_2O$)

200 MHz 1H NMR spectrum in $CDCl_3$

Source: I. L. Reich (digitized hard copy 15-10) g



Problem R-85A ($C_{12}H_{12}Cl_2O$) Determine the structure from the 200 MHz NMR spectrum and the IR spectrum



(a) DBE 6 Interpret the IR spectrum.

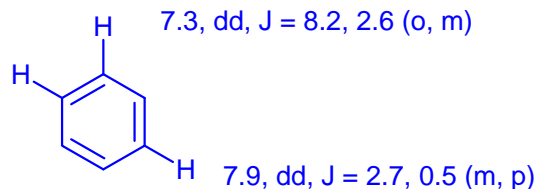
4 3620 free OH 3030 sp^2 CH ($C=C-H$) Strong free OH peak indicates a hindered (tertiary) OH
3470 H-bonded OH No carbonyl

(b) What do you conclude from the NMR signals at δ 7 to δ 8? Draw a part structure, label with δ and J values.

Must be a 1,2,4-trisubstituted benzene

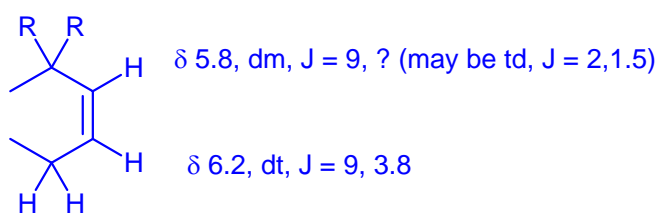
7.4, dd, J = 8.2, 0.5 (o, p)

This accounts for 4 DBE, there is also $C=C$,
so probably a ring in addition

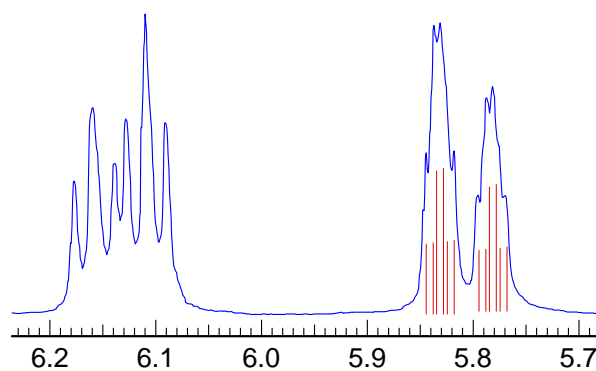


8 (c) What do you conclude from the NMR signals at δ 5.5 to 6.5? Draw a part structure and label with δ and J values.

$R \neq H$

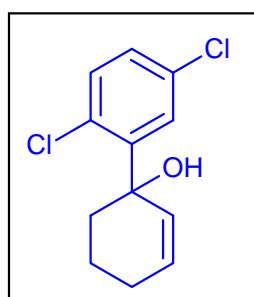


The J_{cis} of 9 Hz means this cannot be a 5 or smaller ring

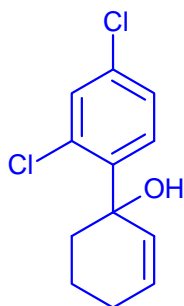


(d) Assign a structure or partial structure to R-85A and identify any structural features you could not establish firmly.

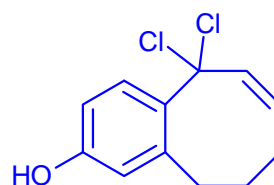
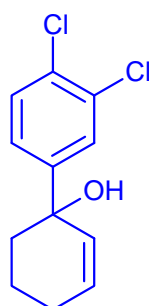
5



Actual structure



Also fit the data



Not a bad alternative structure