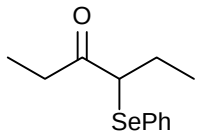
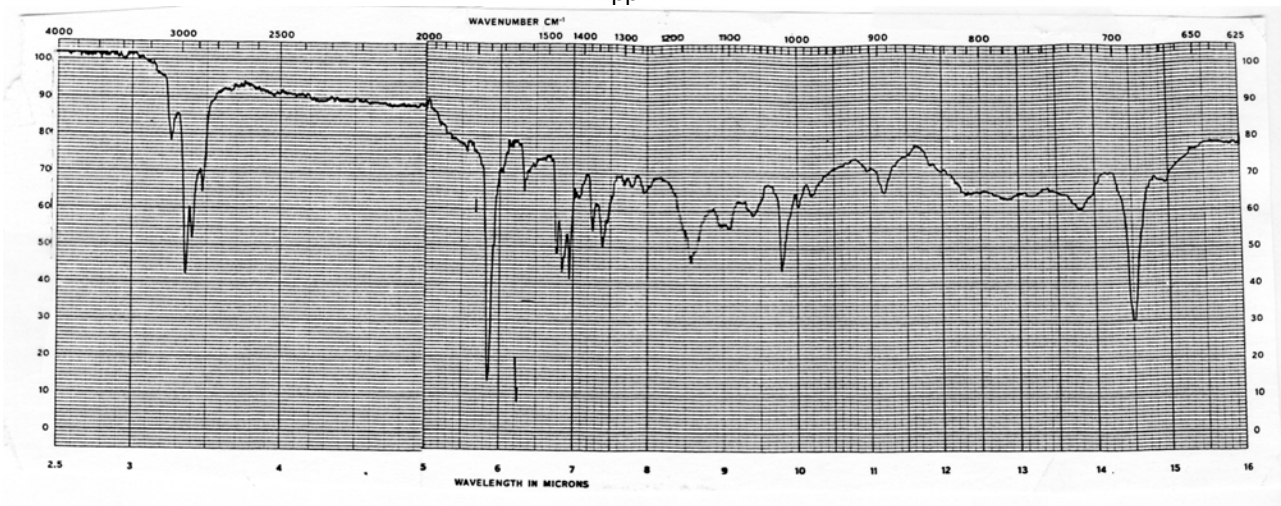
Problem R-10F ($C_{12}H_{16}OSe$)
100 MHz ^1H NMR Spectrum in CCl_4
Source: Hans Reich (digitized hard copy)

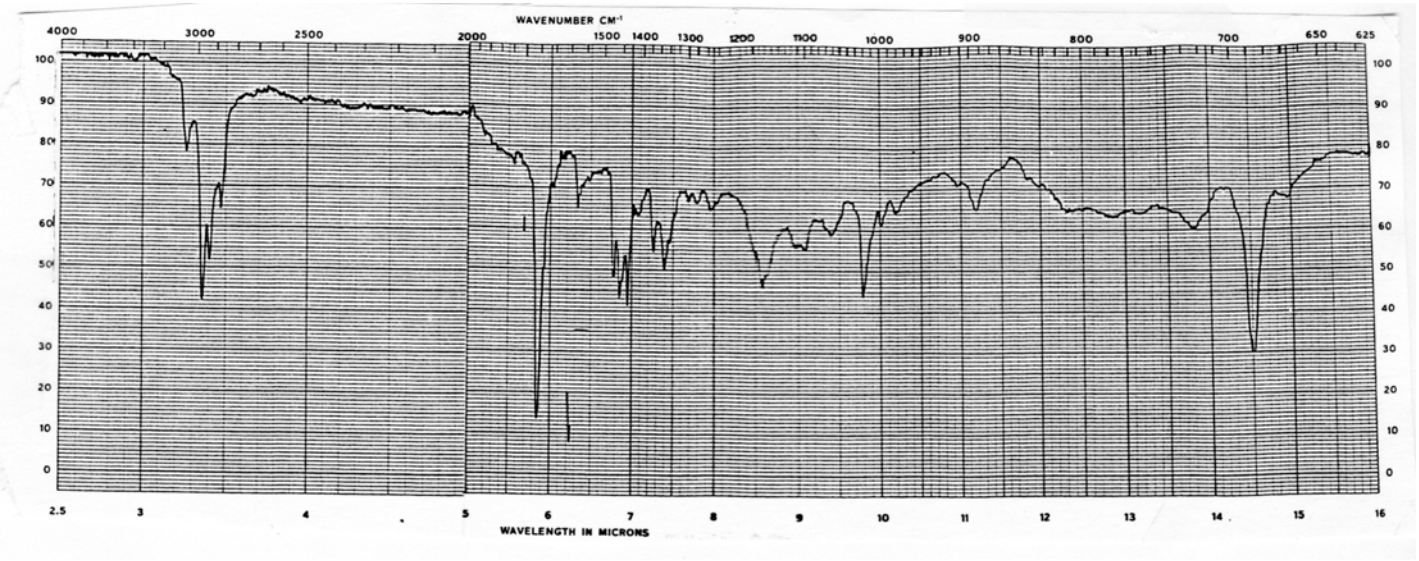




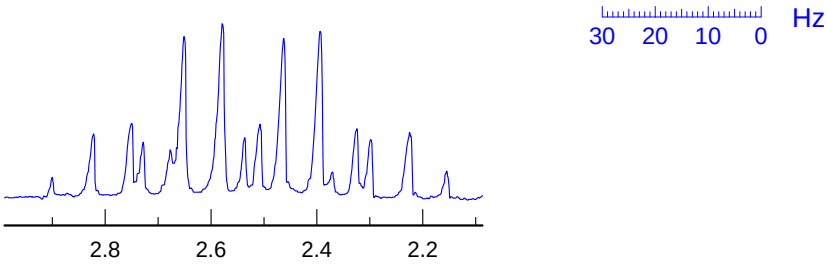
PLT ex-2-2010-11-gq.plt

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 ($C_{12}H_{16}OSe$)
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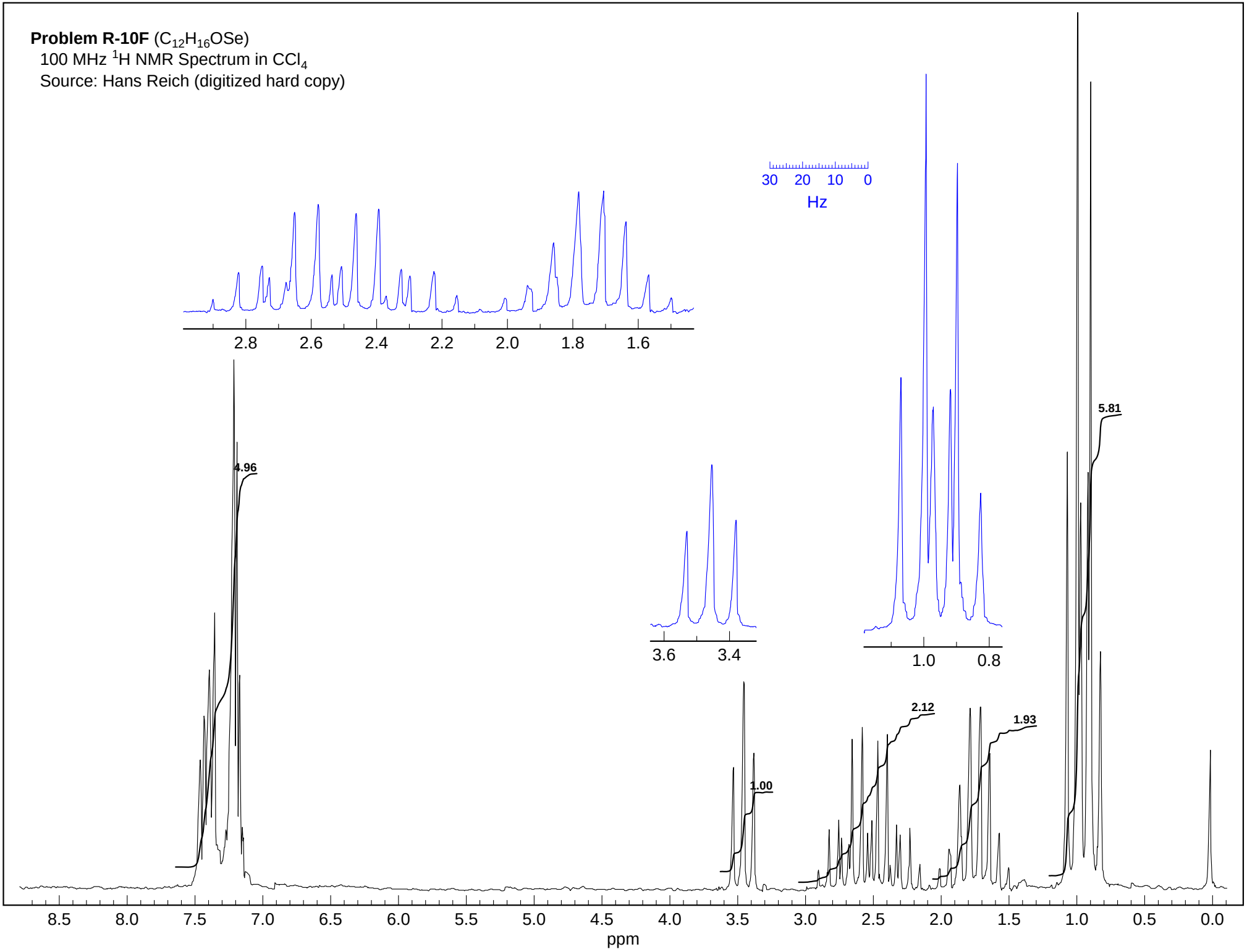


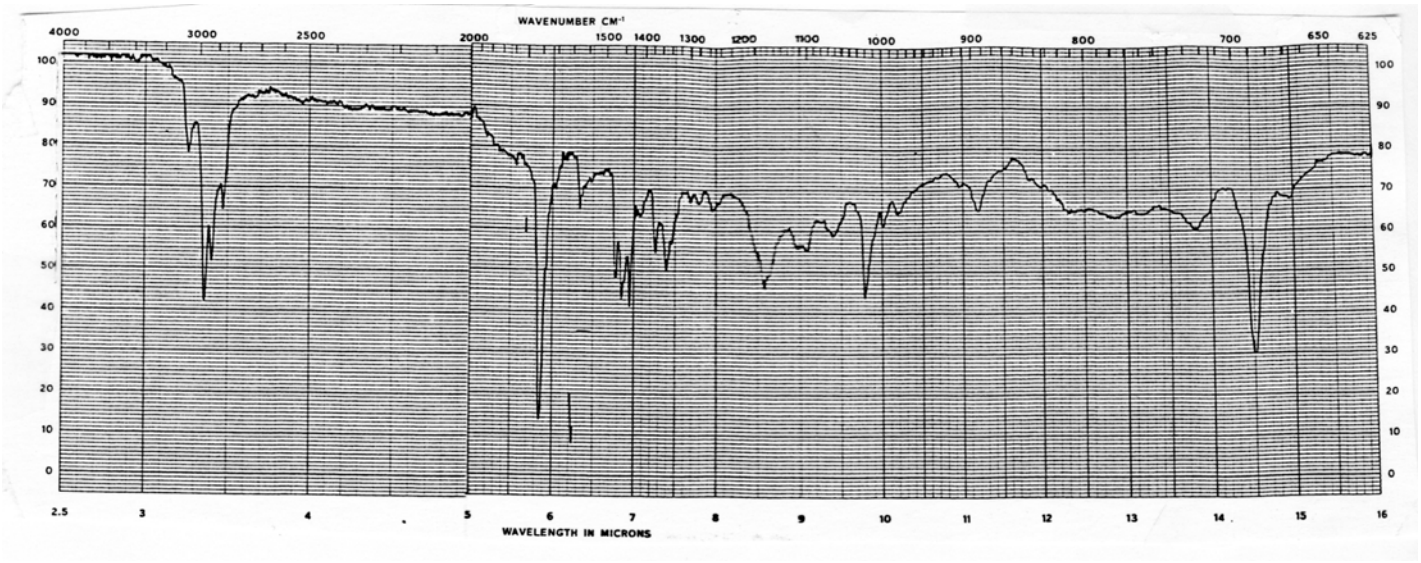
PLT ex-2-2010-11-gq.plt

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.

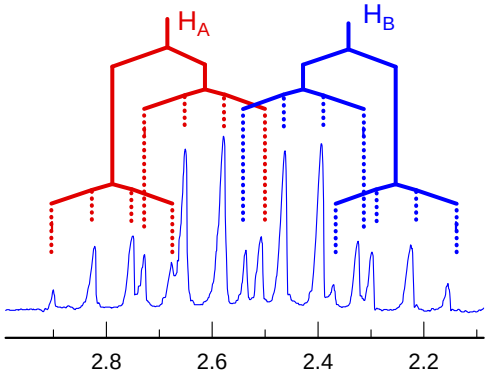
2 (a) DBE 5. (b) Report your analysis of the IR spectrum (CCl_4). List the data and any conclusions you drew from it.

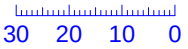
1710 cm^{-1} Ketone No triple bond

4 3050 cm^{-1} Ar-CH



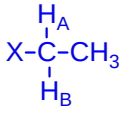
(c) Interpret the 2-proton multiplet at δ 2 to δ 3. What do these signals tell you about the structure. Draw a coupling tree above it to show you understand the multiplet.





This AB part of an ABX_3 pattern (an AB quartet of quartets)

6 cannot be a quartet of quartets - separation is wrong



X can't be O, but could be Se, Ar, or C=O

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

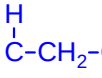
δ 1.0 6H 2 triplets, J = 7 Hz, 2x CH_3CH_2

δ 1.7 2H m (actually AB of ABX_3Y)

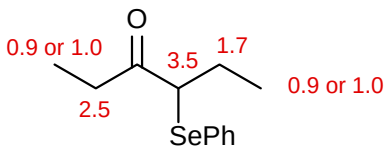
6 δ 3.5 1H t (J=7 Hz) 

CH_3 of ABX_3 above

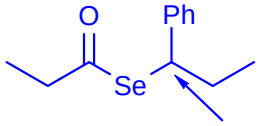
These define this fragment:



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



Without the PhSe hint, other structures (from 2004 exam)



NMR OK, except δ 4.50 (obs 3.5)