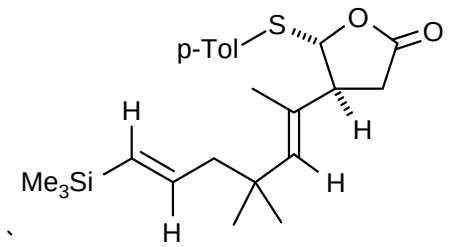
Problem R-10C ($C_{23}H_{34}O_2SSi$)

500 MHz ^1H NMR Spectrum in $CDCl_3$

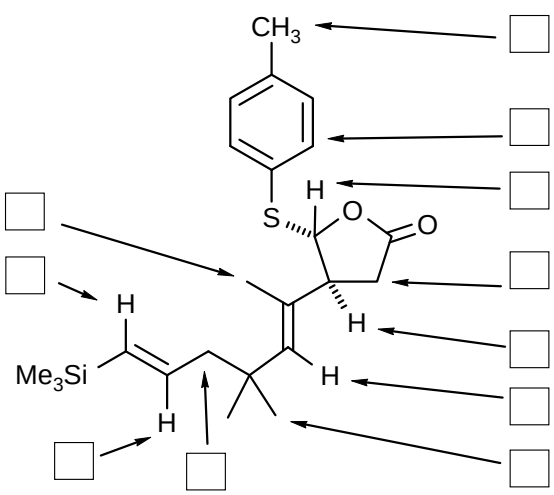
Source: Margaret K. Jones/Burke (Reich digitized hard copy) g

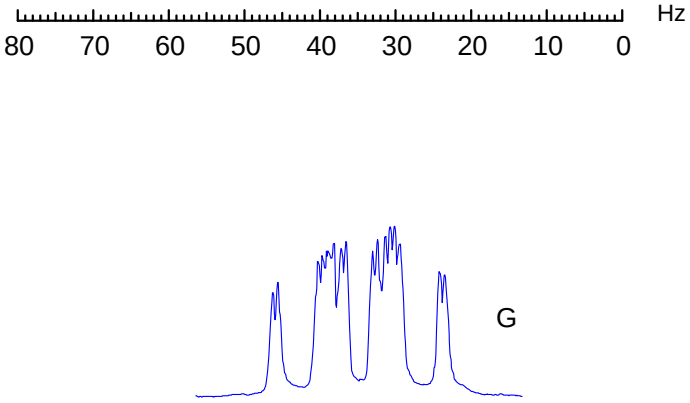


PLT ex-1-2010-11-gq.plt

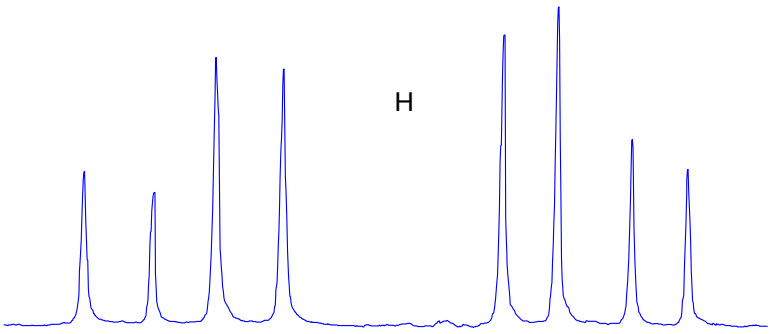
Problem R-10C ($C_{23}H_{34}O_2SSi$) A 500 MHz ^1H spectra is provided.

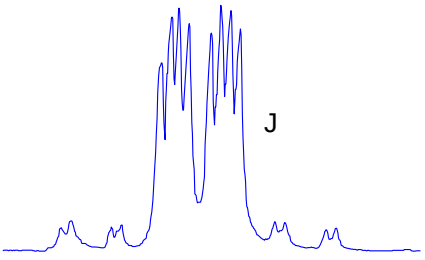
(a) The structure of R-10C is given below. All of the important signals in the ^1H NMR spectrum are labeled (A, B, C etc). Assign the proton signals by placing appropriate labels on the structure. For parts (b), (c) and (d), identify the couplings (e.g. for (b): J_{GX} = 22 Hz, J_{GY} = 32 Hz)





(b) The multiplet at δ 2.9 (**G**) is shown above. How many other protons are coupled to this one?____ Draw a coupling tree for **G** and reort the coupling constants





(c) What kind of pattern is the multiplet at δ 2.5 (**H**)?_____ Draw a coupling tree on the multiplet, label it, and report *J* values.

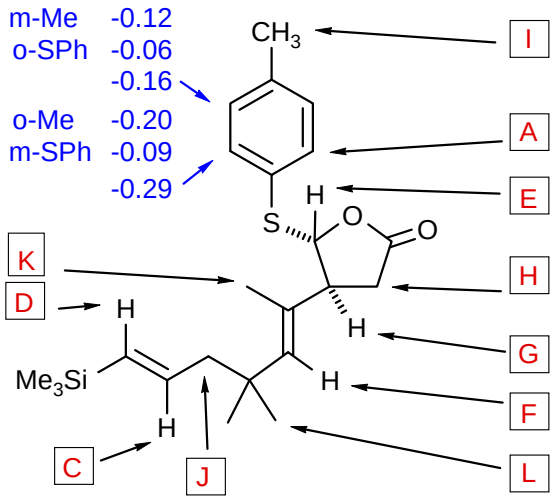
(d) 5 Pt. BONUS question (don't do unless you have spare time): What kind of pattern is the multiplet at δ 2.2 (**J**)? _____ Draw a coupling tree on the multiplet, label it, and report *J* values with assignments.

23

Problem R-10C ($C_{23}H_{34}O_2SSi$) A 500 MHz ^1H spectra is provided.

(a) The structure of R-10C is given below. All of the important signals in the ^1H NMR spectrum are labeled (A, B, C etc). Assign the proton signals by placing appropriate labels on the structure. **For parts (b), (c) and (d), identify the couplings (e.g. for (b): J_{GX} = 22 Hz, J_{GY} = 32 Hz)**

8

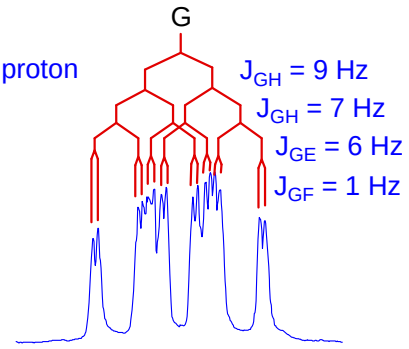


Common errors: switch A/B, H/J, E/F. Decide between A and B with broadening of B by ^4J to CH_3. Select H for a better match with coupling to G, and leaning (weak). Select E for matched coupling with G, and size of coupling.

To make assignments use:
1. Chemical shifts (type of proton
2. Integrations
3. Multiplicity
4. J-values

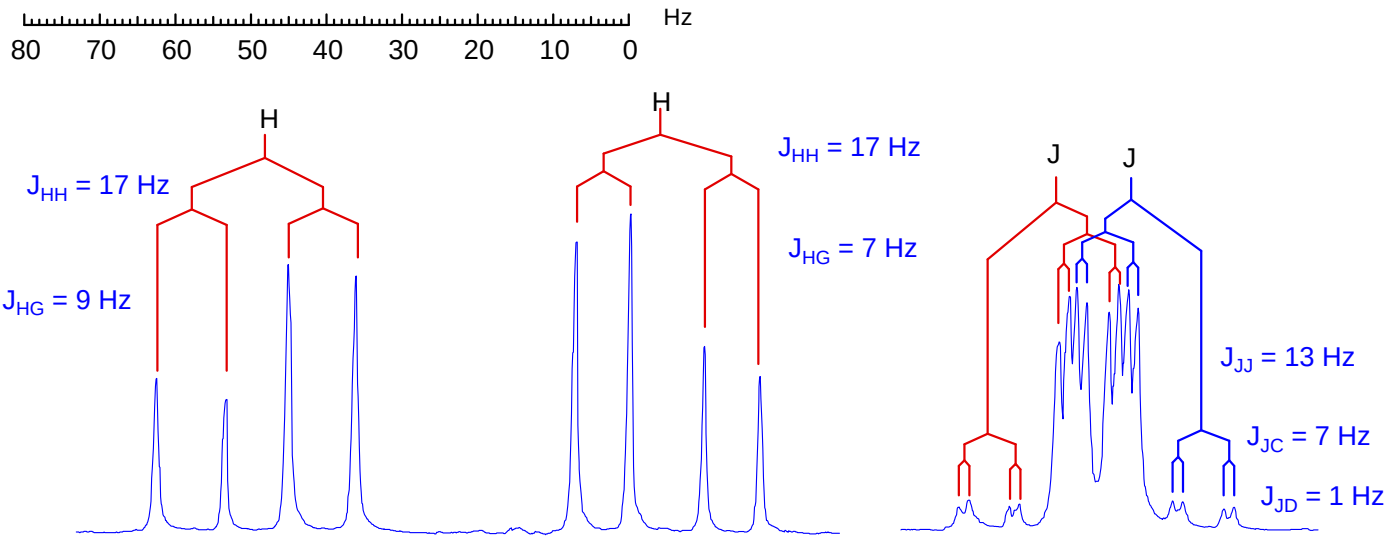
Σ = 23 Hz
End-to-end = 23 Hz

-3 for no J ID



8 (b) The multiplet at δ 2.9 (**G**) is shown above. How many other protons are coupled to this one?___4 Draw a coupling tree for **G** and report the coupling constants

16 lines - therefore coupled to 4 protons



This is AB of ABXY, AB coupled equally to X and Y

7 (c) What kind of pattern is the multiplet at δ 2.5 (**H**)? ABX (AMX) Draw a coupling tree on the multiplet, label it, and report *J* values.

-3 for no J ID

5 (d) 5 Pt. BONUS question (don't do unless you have spare time): What kind of pattern is the multiplet at δ 2.2 (**J**)? AB of ABXY Draw a coupling tree on the multiplet, label it, and report *J* values with assignments.

This is basically an AB pattern (diastereotopic CH_2), each peak of which is split into a dd from coupling to **C** and **D**

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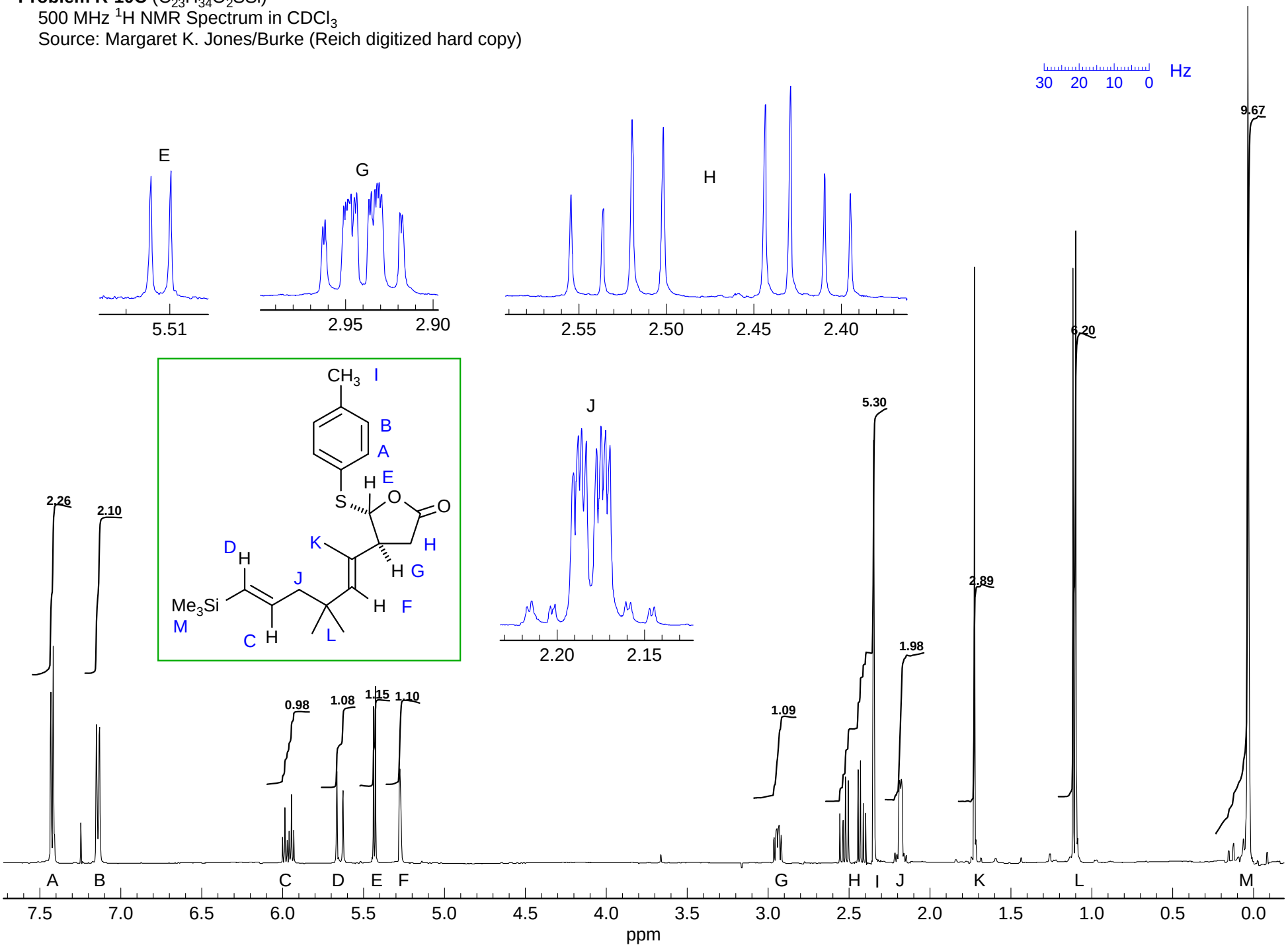

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