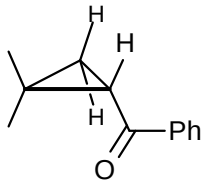
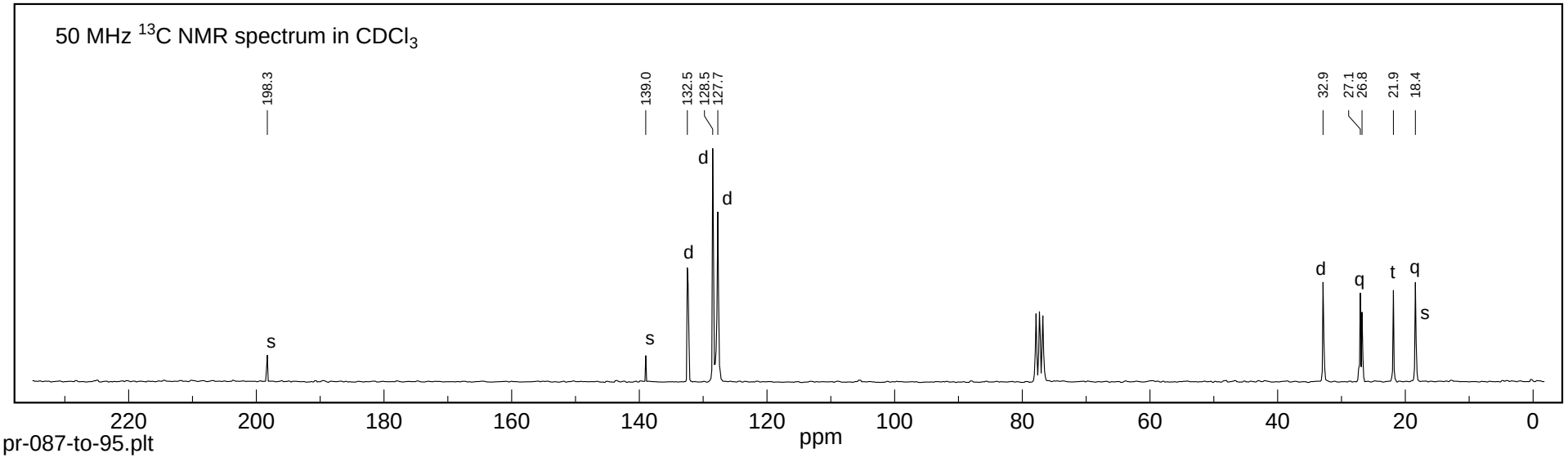
Problem R-94C ($C_{12}H_{14}O$)

200 MHz ^{1}H NMR spectrum in $CDCl_3$

Source: Carl Hoeger (Reich digitized hard copy) g



50 MHz ^{13}C NMR spectrum in $CDCl_3$



PLT pr-087-to-95.plt

Problem R-94C. ($C_{12}H_{14}O$). Determine the structure (or part structure) of **R-94C** from the ^{1}H NMR, ^{13}C NMR and IR spectra provided.

(a) DBE ___ (b) What information can you obtain from the IR spectrum? List the data, and any conclusions you drew from it.

(c) Analyze the ^{1}H NMR signals. For each of the signals listed below report integration, multiplicity and coupling constants to the extent the signals are amenable to first order analysis, and the part structure each corresponds to.

δ 0.9

δ 1.1

δ 1.3

δ 1.5

δ 2.5

δ 7.5

δ 7.9

(c) Interpret the ^{13}C NMR spectrum. Identify what kind of carbon each signal corresponds to, and write possible part structures.

No	ppm	Type of C (e.g. sp^3 CH_2) and/or part structures (e.g. N-CH_2)
1	198.38 (s)	_____
2	139.08 (s)	_____
3	132.30 (d)	_____
4	128.40 (d)	_____
5	127.89 (d)	_____
6	32.82 (d)	_____
7	26.98 (q)	_____
8	26.81 (s)	_____
9	21.96 (t)	_____
10	18.43 (q)	_____

(d) Determine the structure of R-94C. If more than one structure is possible, show them, and circle your best choice.

Problem R-94C ($C_{12}H_{14}O$)

200 MHz ^{1}H NMR spectrum in $CDCl_3$

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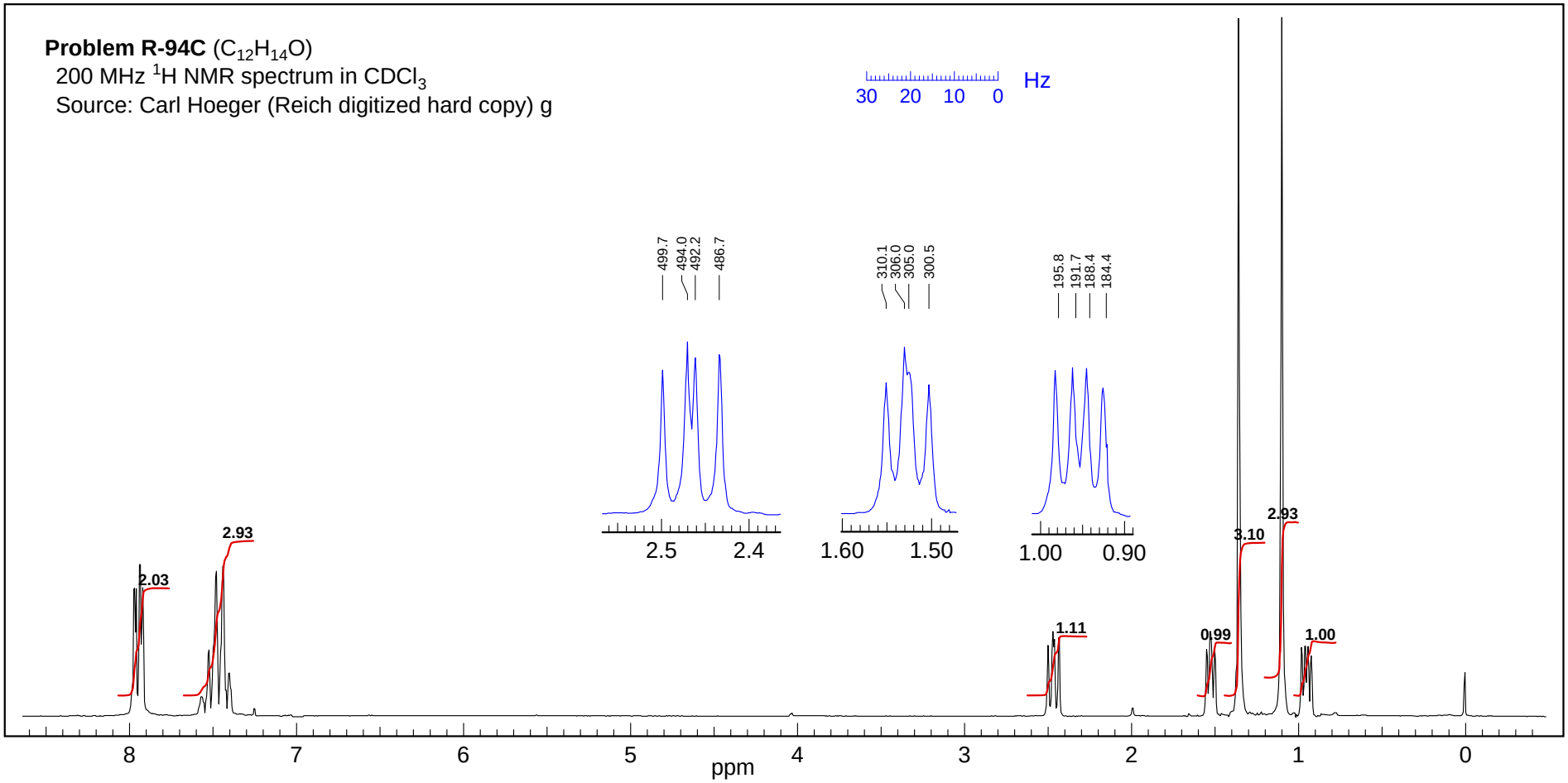
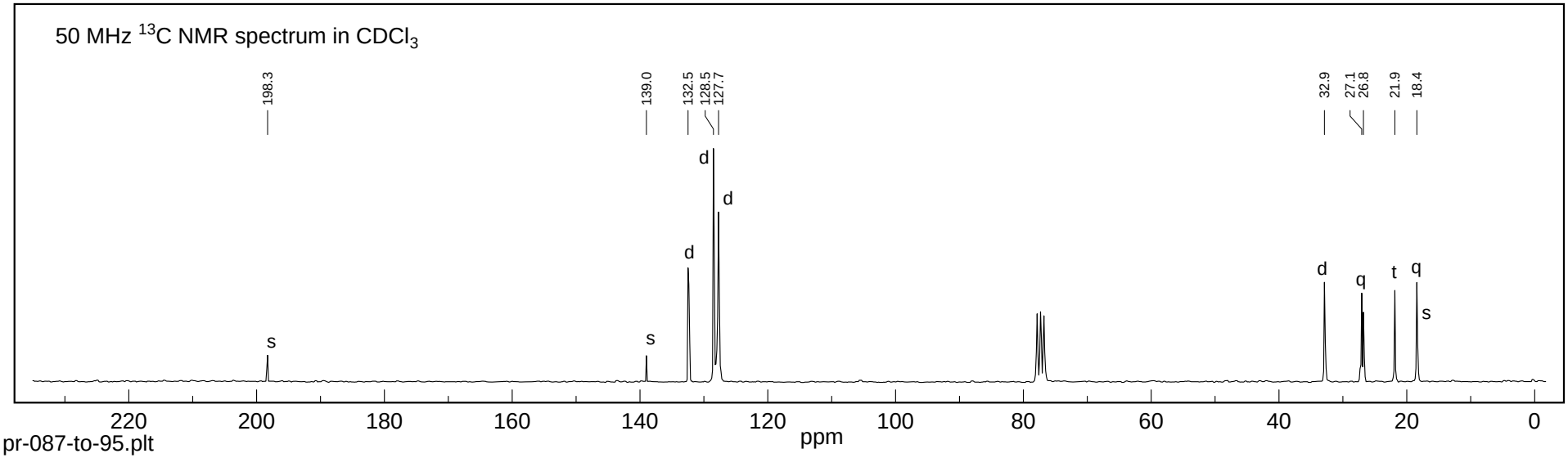


50 MHz ^{13}C NMR spectrum in $CDCl_3$



PLT pr-087-to-95.plt

Problem R-94C. ($C_{12}H_{14}O$). Determine the structure (or part structure) of **R-94C** from the ^{1}H NMR, ^{13}C NMR and IR spectra provided.

(a) DBE 6 (b) What information can you obtain from the IR spectrum? List the data, and any conclusions you drew from it.

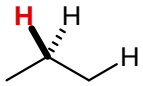
4

1680 cm^{-1} conjugated ketone C=O stretch
3050 cm^{-1} Vinyl/aryl C-H stretch
Absence of peaks above 2300 cm^{-1} - no OH in molecule

(c) Analyze the ^{1}H NMR signals. For each of the signals listed below report integration, multiplicity and coupling constants to the extent the signals are amenable to first order analysis, and the part structure each corresponds to.

5

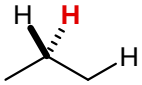
δ 0.9 dd, *J* = 7.7, 3.6 Hz, 1H
Coupled to δ 1.5 and 2.5



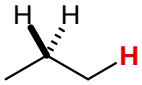
δ 1.1 s, 3H C-C**H**$_3$

δ 1.3 s, 3H C-C**H**$_3$

δ 1.5 dd, *J* = 5.5, 4.3 Hz, 1H
Coupled to δ 0.9 and 2.5

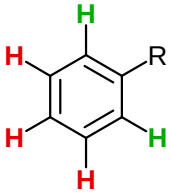


δ 2.5 dd, *J* = 7.4, 5.6 Hz, 1H
Coupled to δ 0.9 and 1.5



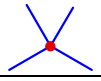
δ 7.5 m, aromatic, 3H, meta and para H

δ 7.9 m, aromatic, 2H, ortho H
R must be electron withdrawing substituent on benzene



The multiplets at δ 0.9, 1.5, 2.5 are an isolated AMX pattern, coupled to nothing else

(c) Interpret the ^{13}C NMR spectrum. Identify what kind of carbon each signal corresponds to, and write possible part structures.

No	ppm	Type of C (e.g. sp^3 CH_2) and/or part structures (e.g. N-CH_2)
1	198.38 (s)	 Not aldehyde
2	139.08 (s)	C (s) ipso aromatic
3	132.30 (d)	C-H aromatic (para)
4	128.40 (d)	C-H aromatic
5	127.89 (d)	C-H aromatic
6	32.82 (d)	 sp^3 tertiary
7	26.98 (q)	C-C**H**$_3$
8	26.81 (s)	 sp^3 quaternary unusually upfield
9	21.96 (t)	sp^3 C-C**H**$_2$-C
10	18.43 (q)	C-C**H**$_3$

ortho and meta double intensity

The 4 signals 127-139 form a monosubstituted benzene

(d) Determine the structure of R-94C. If more than one structure is possible, show them, and circle your best choice.

There is the benzene ring and two more unsaturations - one is the ketone, the other must be a ring.

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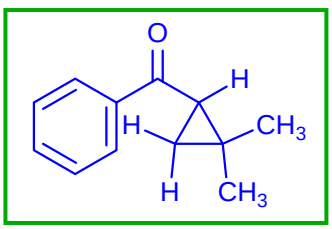
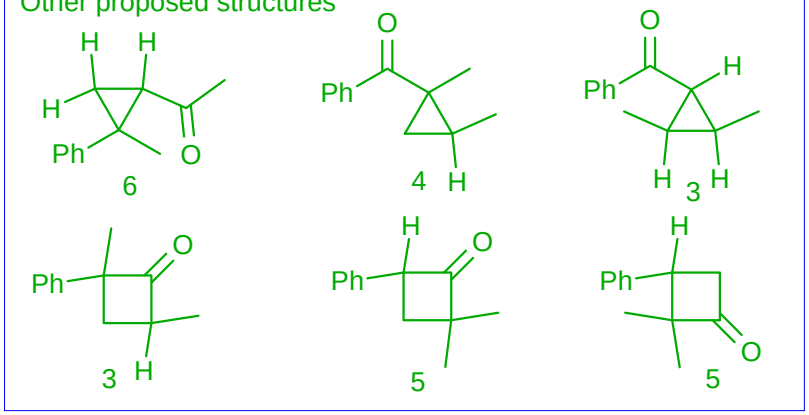


Other proposed structures



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