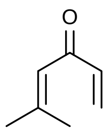
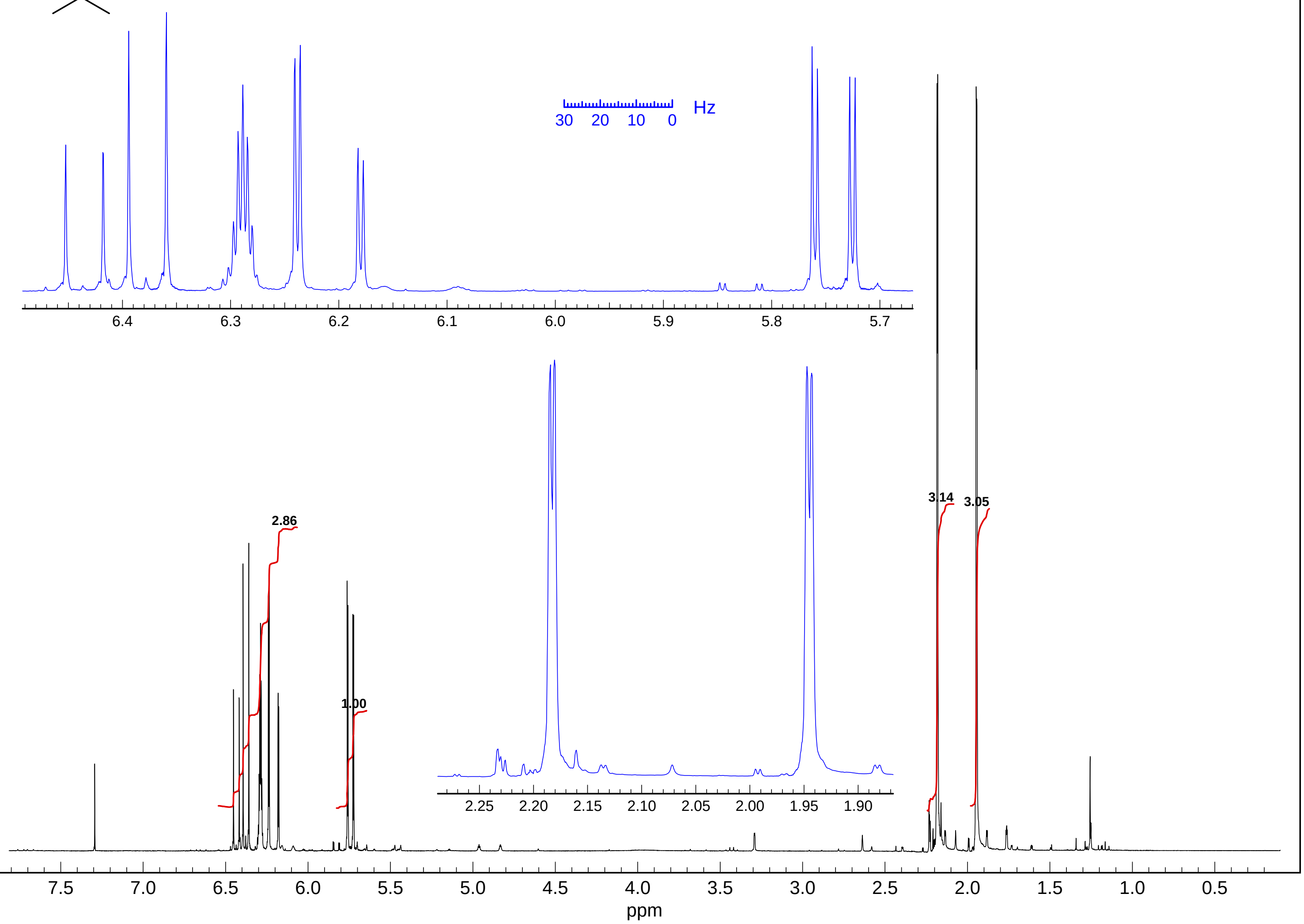
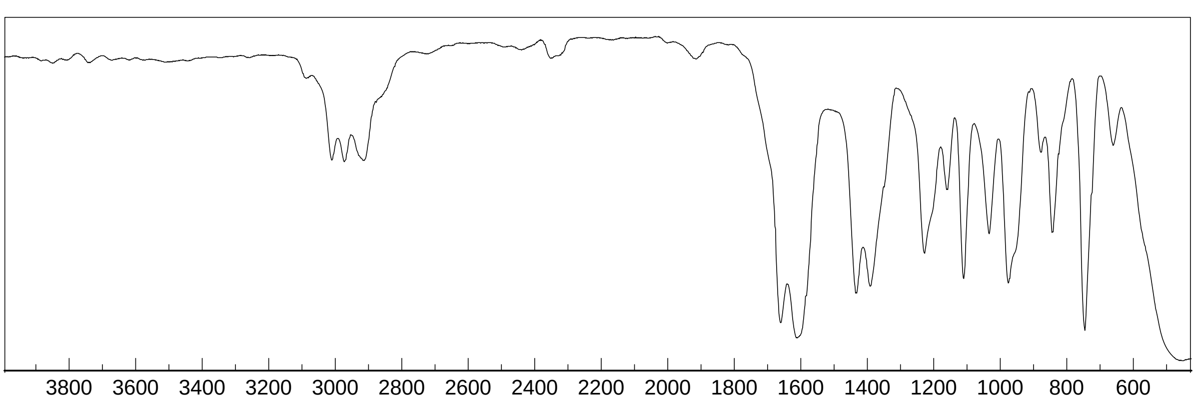
Problem R-03C ($C_7H_{10}O$)
300 MHz ^{1}H NMR Spectrum in $CDCl_3$
Source:Olafs Daugulis/T. Walker/Vedejs 10/26 g



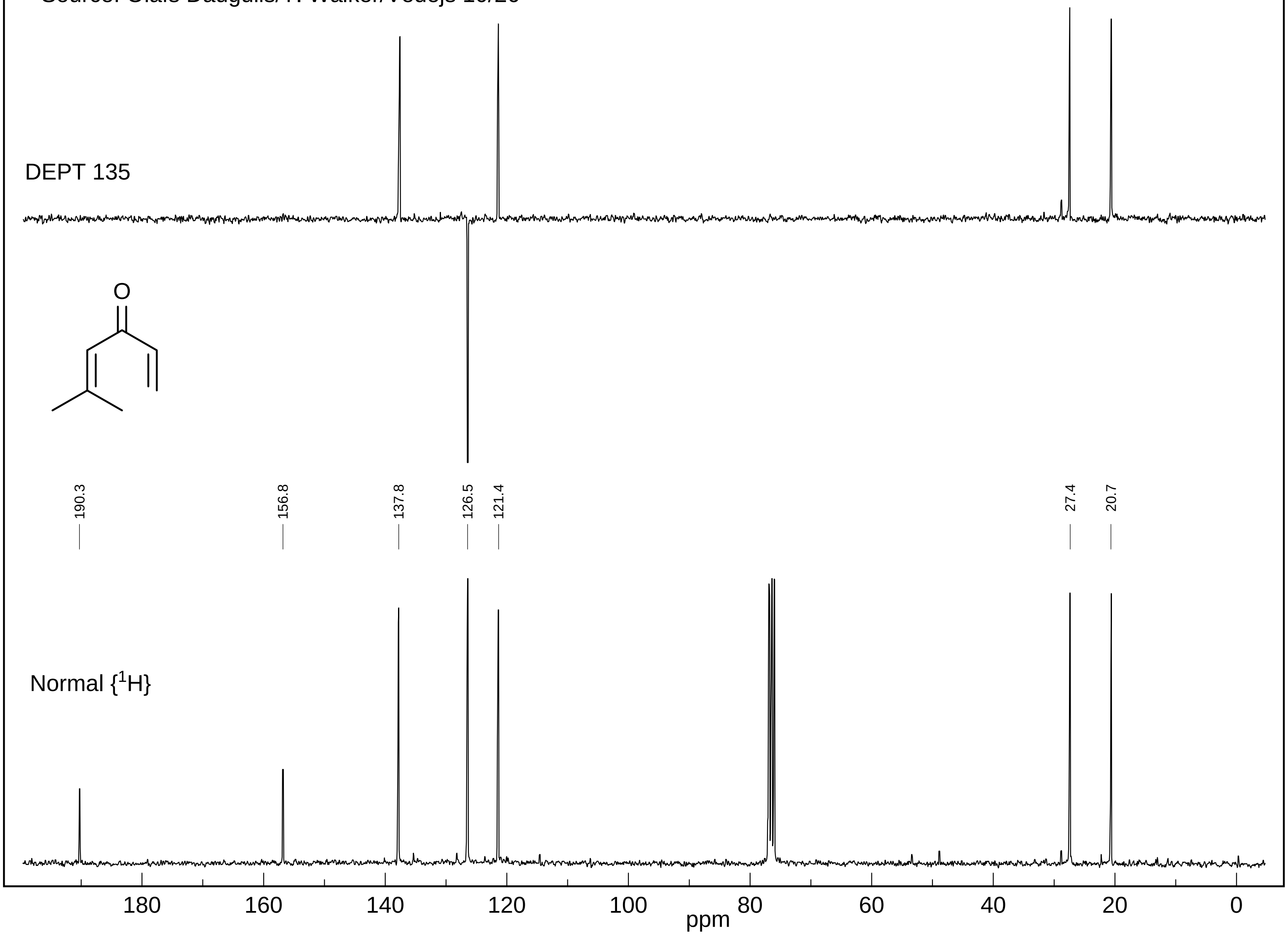


IR Spectrum

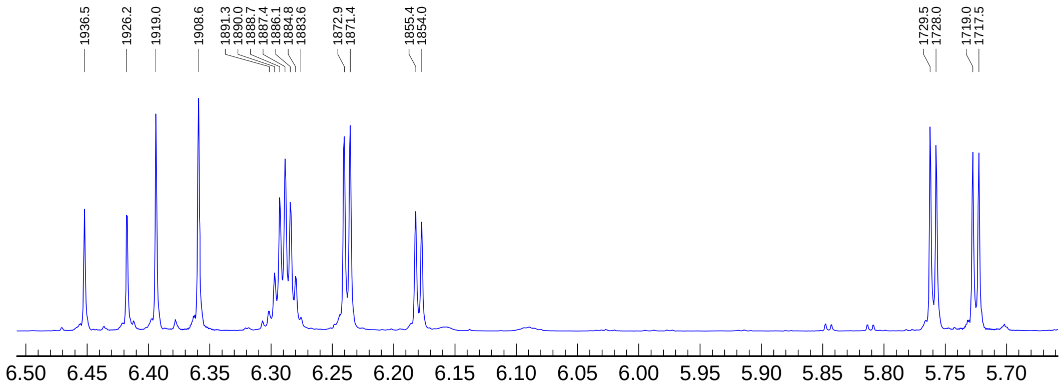


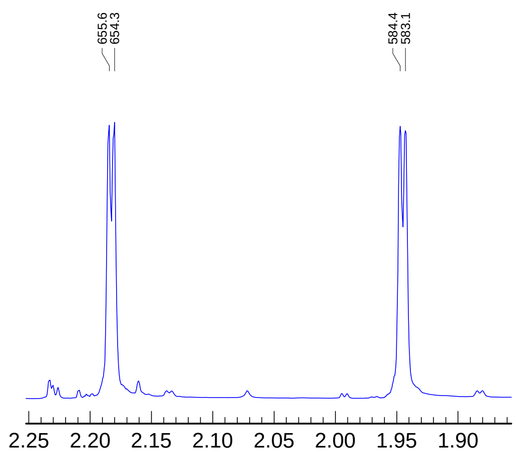
PLT ex-1-2003-gq.plt

Problem R-03C ($C_7H_{10}O$)
75.46 MHz ^{13}C NMR Spectrum in $CDCl_3$
The top spectrum is DEPT 135, with CH_2 negative, CH, CH_3 positive.
Source: Olafs Daugulis/T. Walker/Vedejs 10/26



PLT ex-1-2003-gq.plt



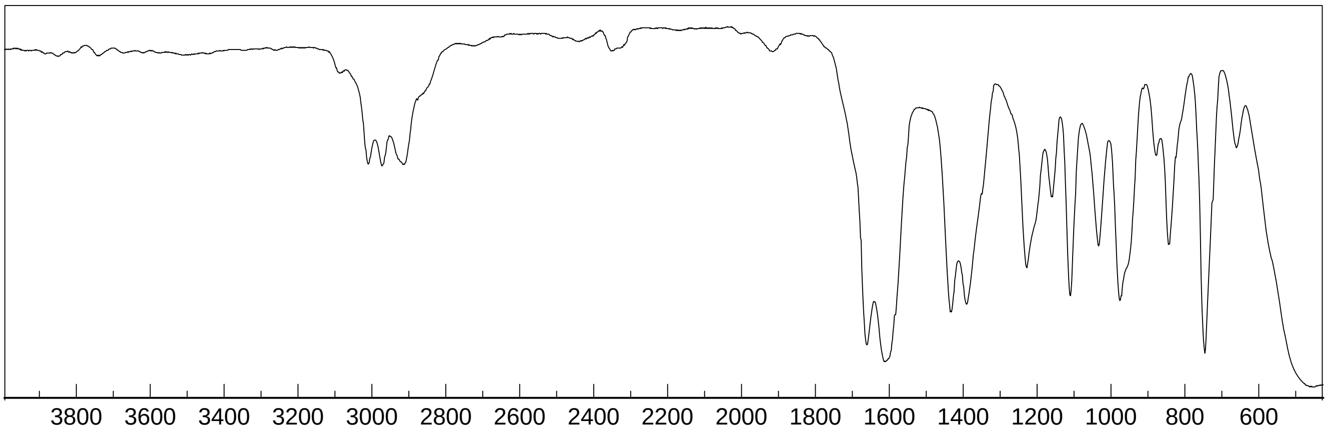


PLT ex-1-2003-gq.plt

Problem R-03C ($C_7H_{10}O$). Determine the structure (or part structure) of R-03C from the ^{1}H NMR, ^{13}C NMR and IR spectra provided.

(a) DBE_______

(b) What information can you obtain from the IR spectrum? Give frequency and assignment.



(c) Interpret the ^{13}C NMR spectrum. The DEPT 135 spectrum shows all CH and CH_3 peaks as positive, and CH_2 peaks negative. Identify what kind of carbon each signal corresponds to, and write possible part structures.

Type of C (e.g. sp^3 CH_2) and/or part structures (e.g. N-CH_2)

δ 21.0 ____

δ 27.8 ____

δ 122.0 ____

δ 127.0 ____

δ 138.2 ____

δ 157.0 ____

δ 190.3 ____

(d) What are the three peaks at δ 77? ____

(e) Assign and analyze the signals between δ 1.9 and 2.2 in the 300 MHz ^{1}H NMR spectrum. Report multiplicity, coupling constants and part structure you could obtain from each signal.

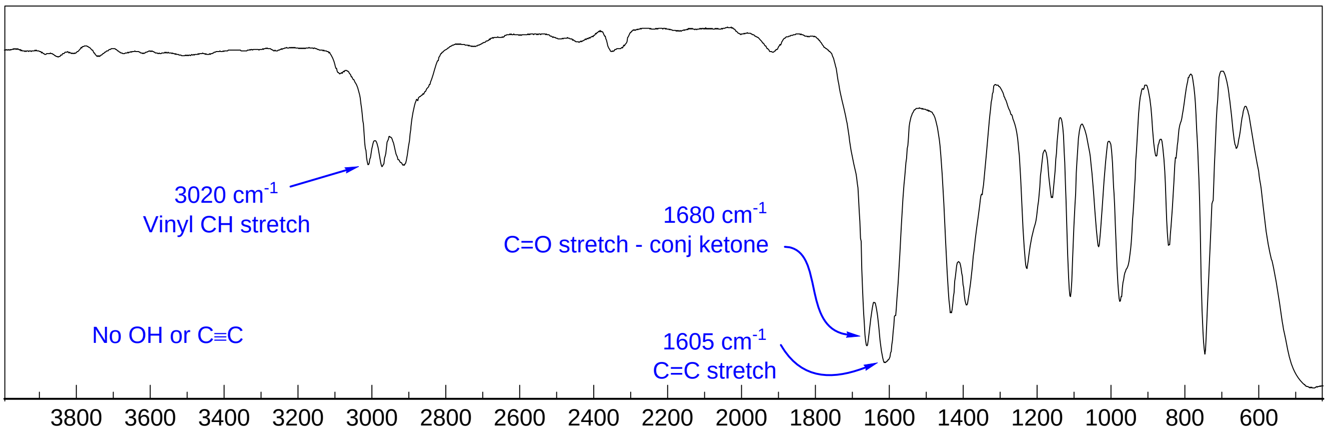
(f) Analyze the multiplets between δ 5.7 and 6.45. Report multiplicity, coupling constants and part structure you could obtain from each signal (in the standard form: e.g., δ 3.9, tq, *J* = 12, 4 Hz, 1H) . You may use first-order analysis.

(g) Draw the structure of **R-03C**. If more than one structure is possible, show them, and circle the one you think fits the data best and give your reasons for choosing it.

Problem R-03C ($C_7H_{10}O$). Determine the structure (or part structure) of R-03C from the ^{1}H NMR, ^{13}C NMR and IR spectra provided.

(a) DBE 3

(b) What information can you obtain from the IR spectrum? Give frequency and assignment.



(c) Interpret the ^{13}C NMR spectrum. The DEPT 135 spectrum shows all CH and CH_3 peaks as positive, and CH_2 peaks negative. Identify what kind of carbon each signal corresponds to, and write possible part structures.

Type of C (e.g. sp^3 CH_2) and/or part structures (e.g. N-CH_2)

δ 21.0	CH_3-C
δ 27.8	CH_3-C
δ 122.0	H–C=C
δ 127.0	CH_2 H_2C=C
δ 138.2	H–C=C
δ 157.0	>C=C Quaternary
δ 190.3	O=C Conjugated ketone

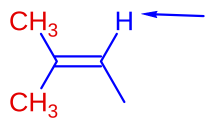
(d) What are the three peaks at δ 77? These are the $CDCl_3$ peaks (C split by D, *I* = 1)

PLT ex-1-2003-gq.plt

(e) Assign and analyze the signals between δ 1.9 and 2.2 in the 300 MHz ^{1}H NMR spectrum. Report multiplicity, coupling constants and part structure you could obtain from each signal.

Two CH_3 groups, each split into a d, J = 1.3 Hz

Chemical shifts suggests CH_3 on double bond or aryl ring



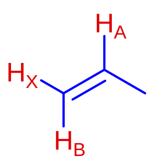
Coupling suggests ^{4}J allylic

(f) Analyze the multiplets between δ 5.7 and 6.45. Report multiplicity, coupling constants and part structure you could obtain from each signal (in the standard form: e.g., δ 3.9, tq, J = 12, 4 Hz, 1H) . You may use first-order analysis.

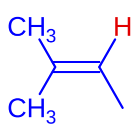
δ 6.40 dd, J = 17.5, 10.4 Hz. A part of ABX (trans and cis vivyl coupling)

δ 6.21 dd, J = 17.5, 1.5 Hz. B part of ABX (trans and gem)

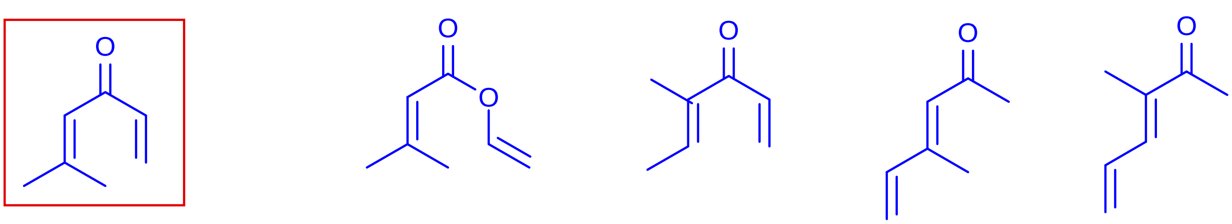
δ 5,74 dd, J = 10.4, 1.5 Hz. X part of ABX (cis and gem)



δ 6.29, septet, J = 2 Hz: vinyl proton split by 6 protons with small J - coupled to both CH_3 groups



(g) Draw the structure of **R-03C**. If more than one structure is possible, show them, and circle the one you think fits the data best and give your reasons for choosing it.



+ 10 other structures