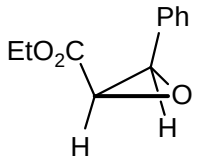
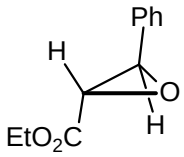
Problem R-12G ($C_{11}H_{12}O_3$).
200 MHz ^{1}H NMR Spectrum in $CDCl_3$.
Source: Tom Fleck/Vedejs (digitized hard copy) g



PLT ex-2-2012-13-gq.plt

Problem R-12H ($C_{11}H_{12}O_3$).
200 MHz ^{1}H NMR Spectrum in $CDCl_3$.
Source: Tom Fleck/Vedejs (digitized hard copy) g

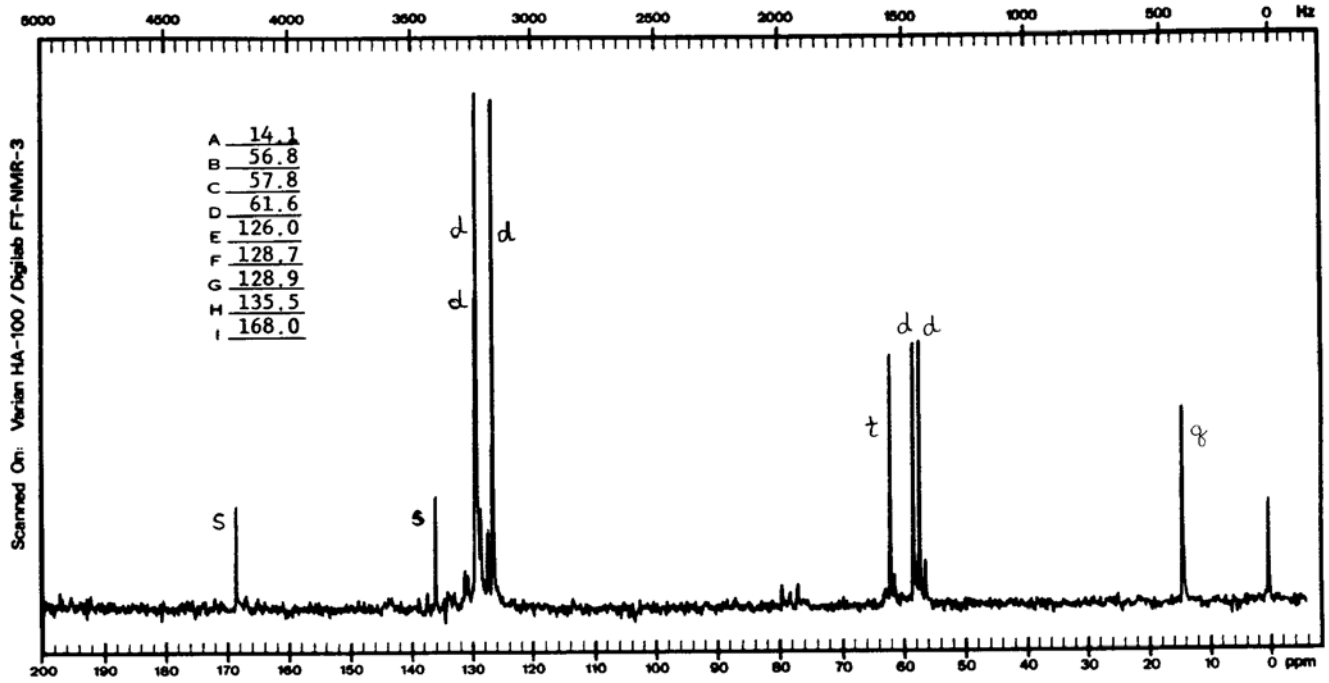


PLT ex-2-2012-13-gq.plt

Problem R-12H ($C_{11}H_{12}O_3$).

25 MHz ^{13}C NMR Spectrum in $CDCl_3$.

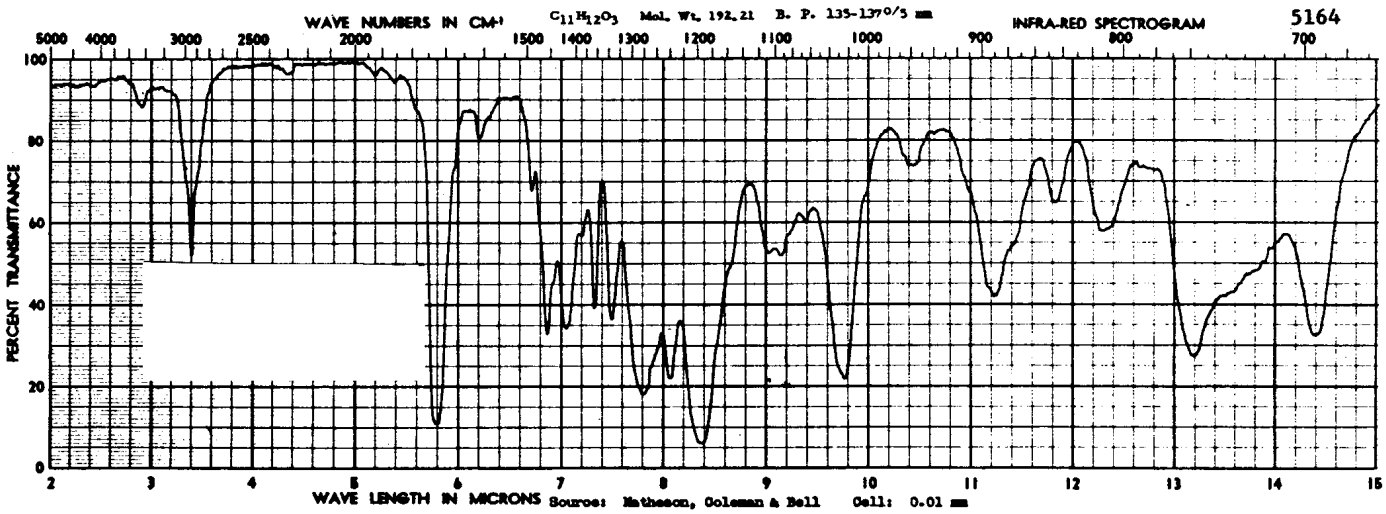
Source: Sadtler



Problem R-12H ($C_{11}H_{12}O_3$).

IR Spectrum neat.

Source: Sadtler



PLT ex-2-2012-13-gq.plt

Problem R-12G ($C_{11}H_{12}O_3$). **R-12G** and **R-12H** are two stereoisomers. For R-12G only the ^1H spectrum is provided, R-12H has in addition ^{13}C and IR spectra. The compounds each contain a Ph group.

(a) DBE _____

(b) What can you learn from the IR spectrum of **R-12H**?

(b) Identify significant peaks in the ^{13}C NMR spectrum of **R-12H** and describe the structural information you obtained from them.

(c) Draw the structures of **R-12G** and **R-12H** below. Label the structures with ^1H chemical shifts and coupling constants.

(e) What feature(s) of the spectra allowed you to make the distinction between the isomers?

Problem R-12G ($C_{11}H_{12}O_3$). **R-12G** and **R-12H** are two stereoisomers. Only the ^1H spectrum of R-12G is provided, R-12H has in addition ^{13}C and IR spectra. The compounds each contain a Ph group.

2 (a) DBE 6

(b) What can you learn from the IR spectrum of **R-12H**?

1730 cm^{-1} possible ester C=O, not 4 or 5 ring

1490, 1460, 1420 aromatic

No OH stretch (not acid or alcohol)

4

1030 cm^{-1} C-O

(b) Identify significant peaks in the ^{13}C NMR spectrum of **R-12H** and describe the structural information you obtained from them.

14.2: CH_3

61.6: CH_2-O

57.8, 61.6: two CH-O

6

135.5: quat aromatic

128.9, 128,7, 126.0: aromatic p, o, m

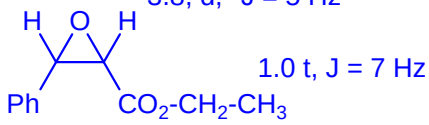
168.0: Ester carbonyl

(c) Draw the structures of **R-12G** and **R-12H** below. Label the structures with ^1H chemical shifts and coupling constants.

Assign the downfield epoxide proton to the PhCH because it is a little broader (not so tall) due to coupling to Ph protons Also, α-Ph (CH) is 1.35, α-CO_2R (CH) is 0.95.

4.25, d, ^3J = 5 Hz

3.8, d, ^3J = 5 Hz



1.0 t, J = 7 Hz

6

4.0, AB of ABX_3

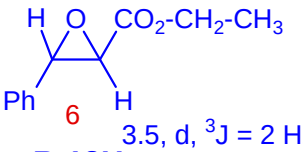
10

R-12G

4.05, d, ^3J = 2 Hz

4.25, AB of ABX_3

1.3, t, J = 7 Hz

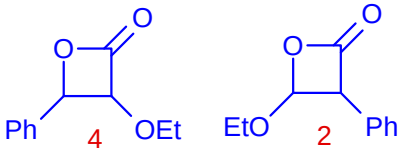


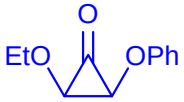
6

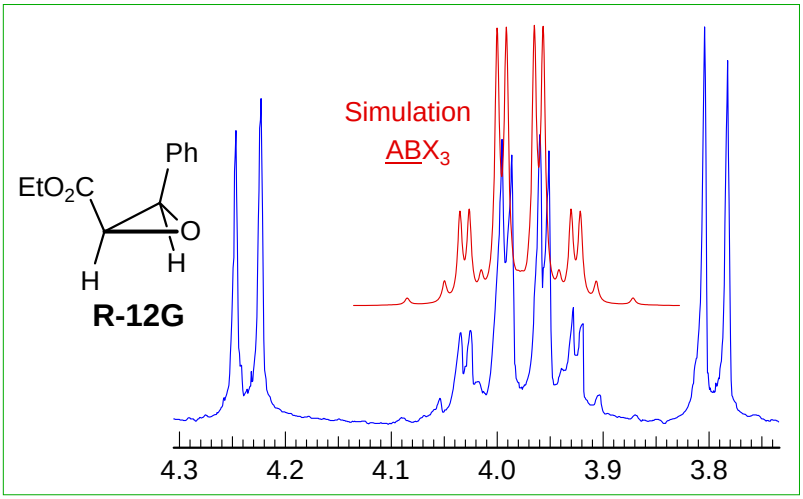
3.5, d, ^3J = 2 Hz

R-12H

Other structures







(e) What feature(s) of the spectra allowed you to make the distinction between the isomers?

In 3-membered rings J_{cis} is <u>always</u> larger than J_{trans} for a given system

3

In 4-membering rings J_{cis} is <u>usually</u> larger than J_{trans}