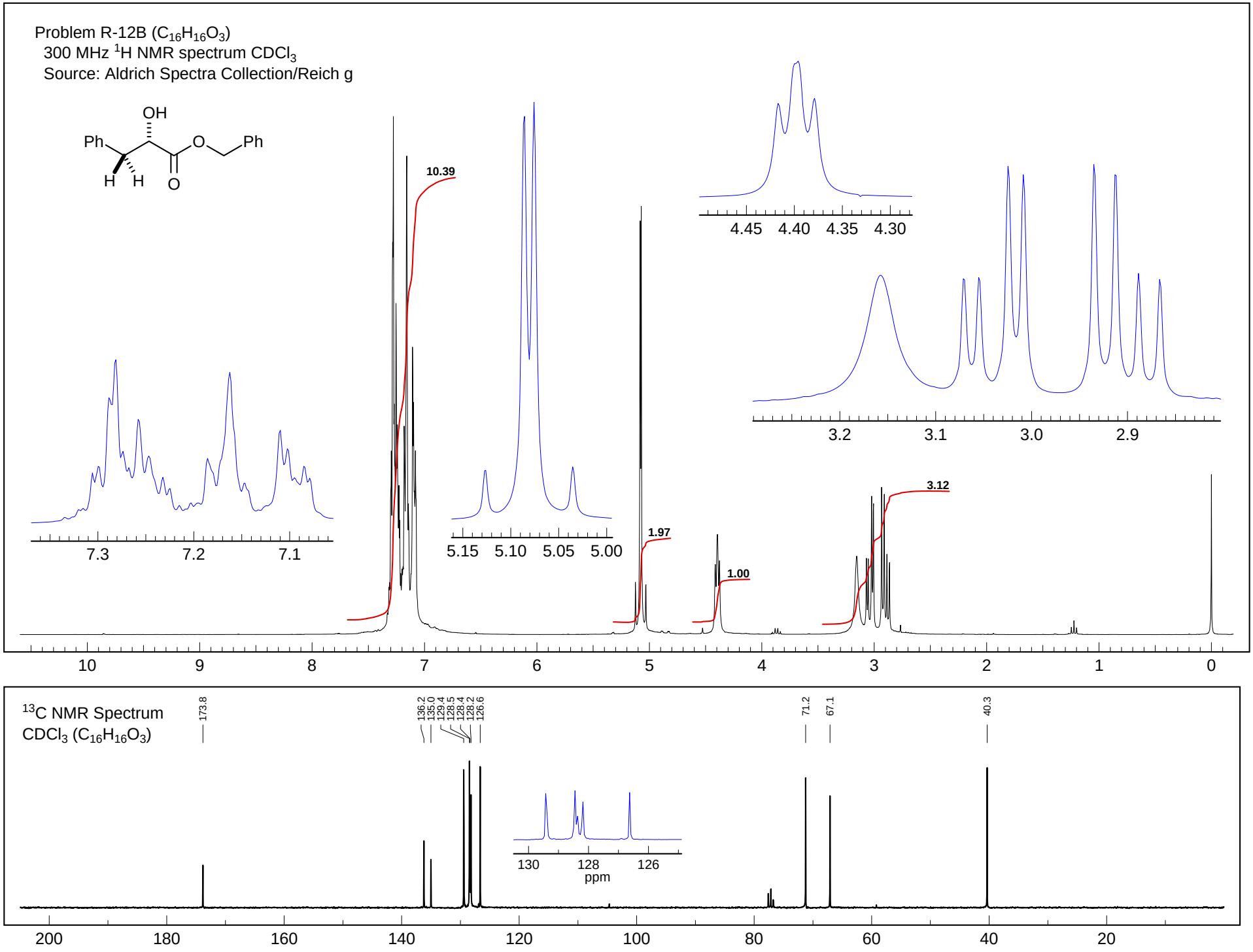
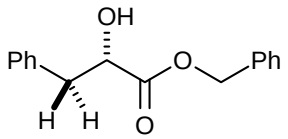
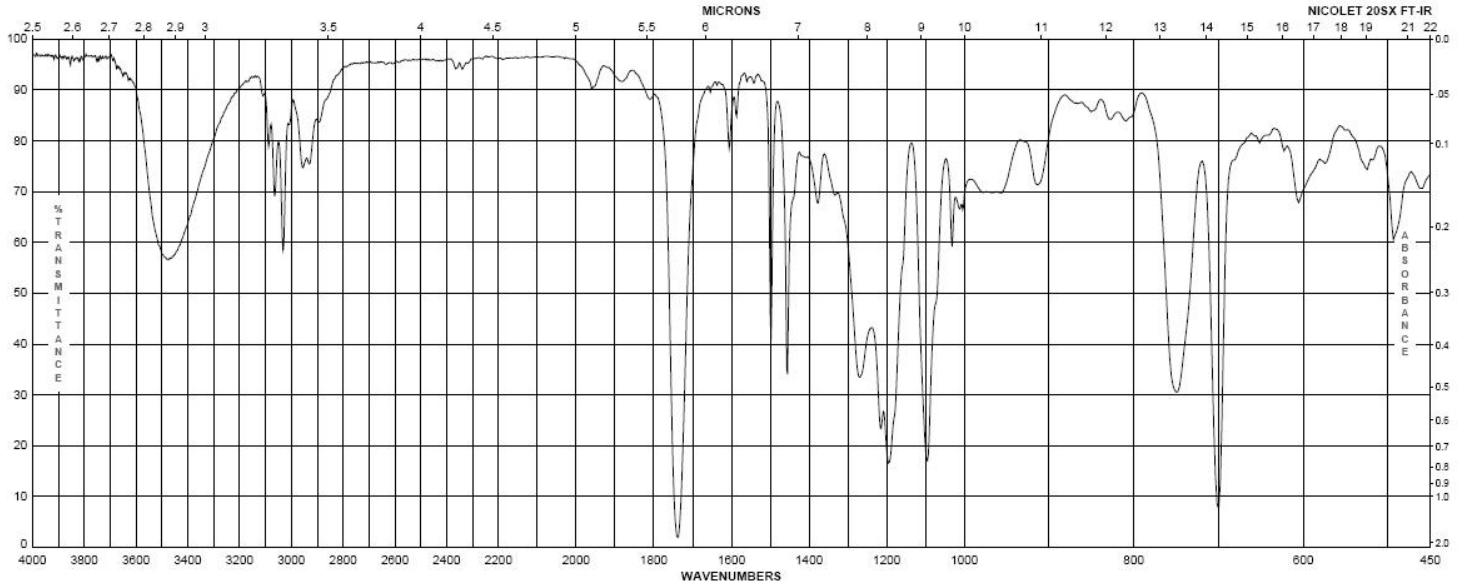


PLT ex-1-2012-13-gq.plt

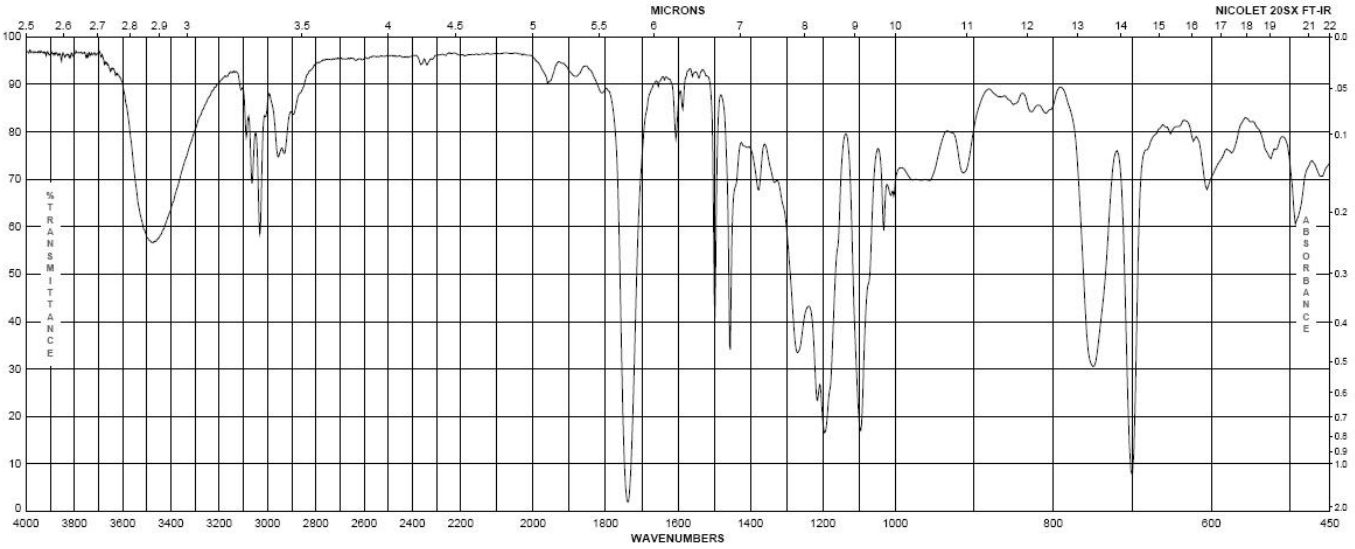




PLT ex-1-2012-13-gq.plt

Problem R-12B ($C_{16}H_{16}O_3$). Determine the structure (or part structure) of **R-12B** from the IR, ^{1}H NMR and ^{13}C NMR spectra provided.

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



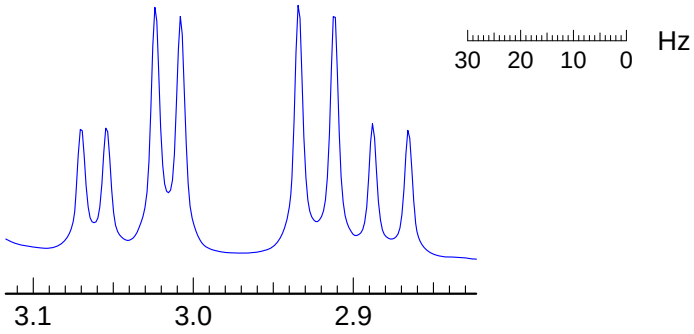
(c) Interpret the ^{13}C NMR spectrum. The multiplicity of each signal is given on the spectrum. Identify what kind of carbon each signal corresponds to (be as specific as possible) and write likely part structures.

Type of C (e.g. sp^3 $\underline{C}H_2$) and/or part structures (e.g. N-$\underline{C}H_2$)

ppm			
40.3	_____	128.5	_____
67.1	_____	129.4	_____
71.2	_____	135.0	_____
126.6	_____	136.2	_____
128.2	_____	173.8	_____
128.4	_____		

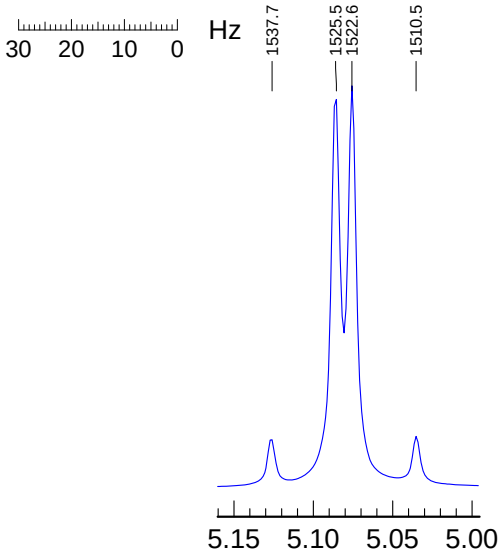
/

(d) Analyze the 2-proton multiplet between δ 2.8 and 3.1 (reproduced below). Draw a coupling tree and report coupling constants (in the standard form: e.g., δ 3.9, tq, J = 12, 4 Hz, 1H) and part structure you could obtain from the signal. You may use first-order analysis.



What kind of pattern is this?_____ What other signal is coupled to these protons?_____

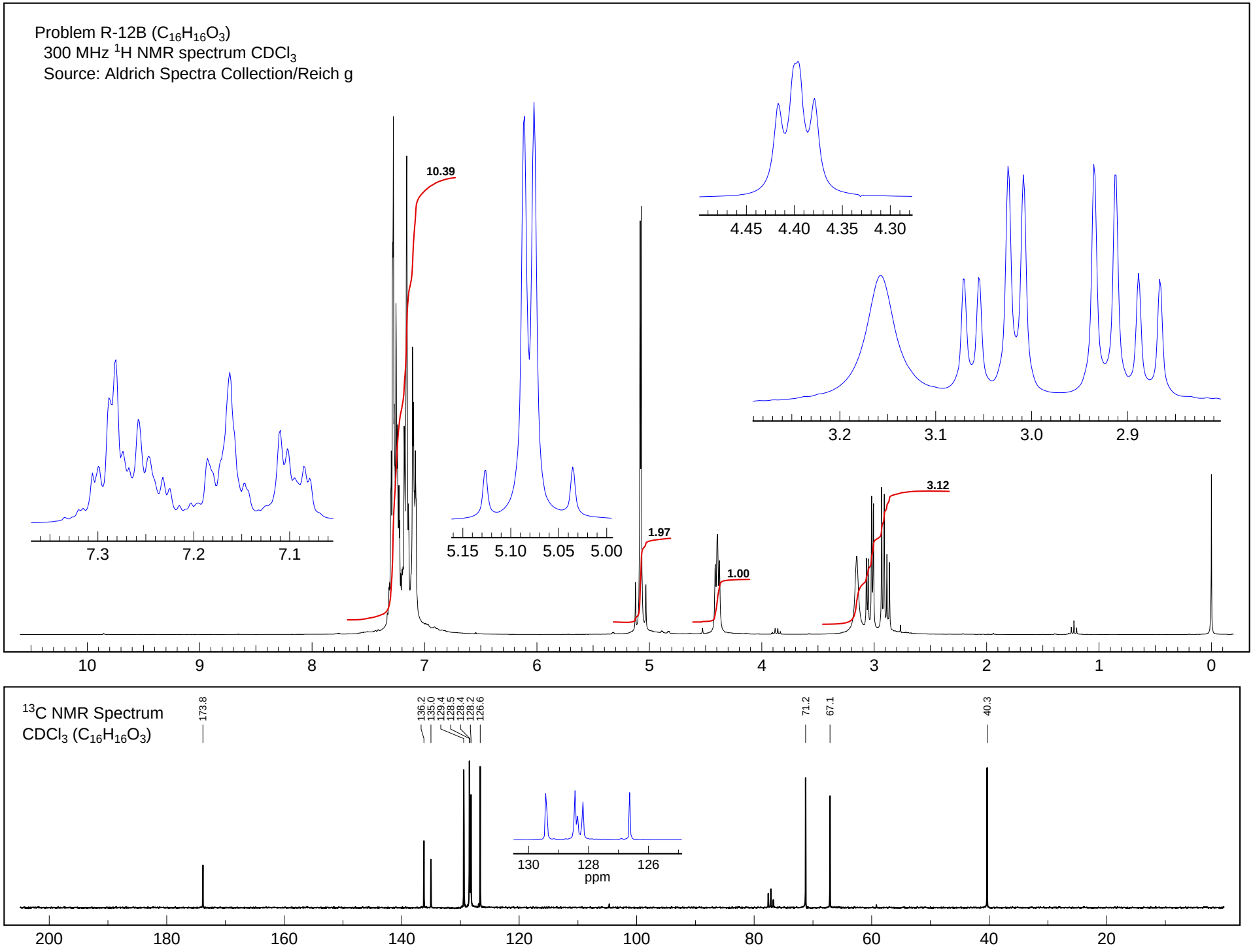
(e) Analyze the two-proton multiplet between δ 5.0 and 5.2 in the ^{1}H NMR spectrum. The multiplet is reproduced below. Draw a coupling tree and report exact coupling(s) and chemical shifts, and a part structure.



What kind of pattern is this?_____

(e) Show a structure for **R-12B**. If there is more than one possibility, circle your best choice.

(f) Do a chemical shift calculation (from methane as model) of the carbon in your structure you have assigned the signal at δ 40.3. Show parameters you used.

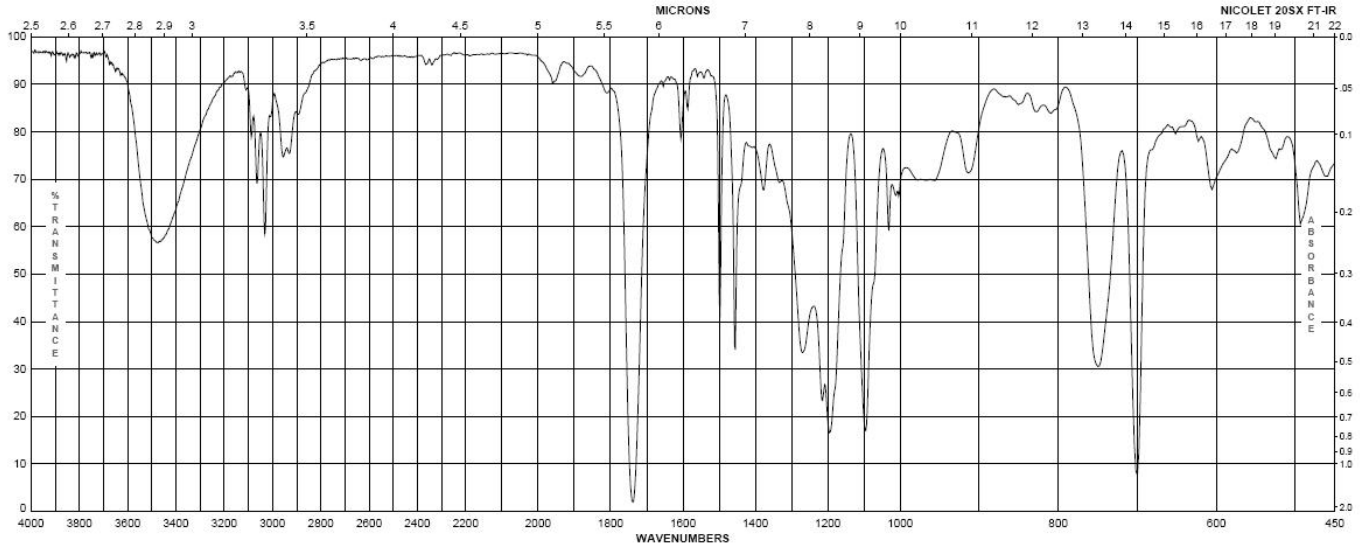


PLT ex-1-2012-13-gq.plt

Problem R-12B ($C_{16}H_{16}O_3$). Determine the structure (or part structure) of **R-12B** from the IR, ^{1}H NMR and ^{13}C NMR spectra provided.

2

(a) DBE 9 (b) What information can you obtain from the IR spectrum? Give frequency and assignment.



4

3470 cm^{-1} OH stretch
3040, 3060 sp^2 C-H stretch (aromatic C-H)
1740 cm^{-1} C=O stretch, probably of an ester

(c) Interpret the ^{13}C NMR spectrum. The multiplicity of each signal is given on the spectrum. Identify what kind of carbon each signal corresponds to (be as specific as possible) and write likely part structures.

Type of C (e.g. sp^3 $\underline{C}H_2$) and/or part structures (e.g. N-$\underline{C}H_2$)

ppm		ppm	
40.3	sp^3 CH_2	128.5	sp^2 CH 3x?
67.1	sp^3 OCH	129.4	sp^2 CH 2x
71.2	sp^3 OCH_2	135.0	sp^2 C
126.6	sp^2 CH 2x	136.2	sp^2 C
128.2	sp^2 CH 2x	173.8	CO_2R
128.4	sp^2 CH		

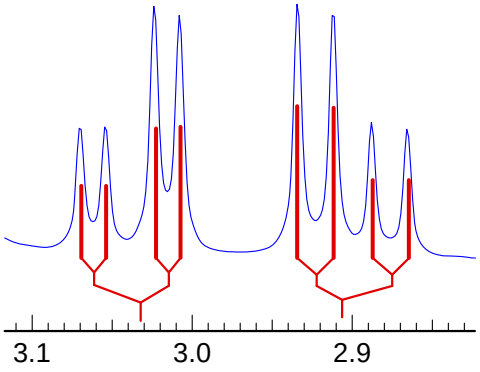
4

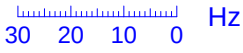
/

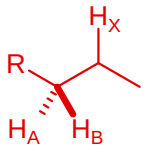
(d) Analyze the 2-proton multiplet between δ 2.8 and 3.1 (reproduced below). Draw a coupling tree and report coupling constants (in the standard form: e.g., δ 3.9, tq, J = 12, 4 Hz, 1H) and part structure you could obtain from the signal. You may use first-order analysis.

6

δ 3.03 dd, J = 14, 4.5 δ 2.91 dd, J = 14, 6.5







From the chemical shift
R is likely to be C=O or Ph

What kind of pattern is this? AB of ABX What other signal is coupled to these protons? 4.4 δ

(e) Analyze the two-proton multiplet between δ 5.0 and 5.2 in the ^{1}H NMR spectrum. The multiplet is reproduced below. Draw a coupling tree and report exact coupling(s) and chemical shifts, and a part structure.

6

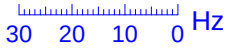
J_{AB} = 12.2

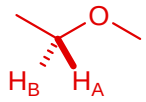
c=(5+3)/2 = 1524.08

$\Delta\nu_{ab}$ = sqrt((4-1)(3-2)) = 8.9

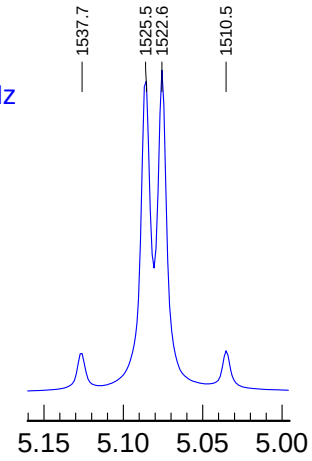
$c \pm \nu_{ab}/2$ = 1528.6 1519.6

δ_A, δ_B = 5.095 5.065





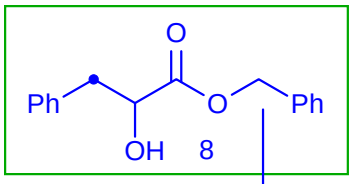
Must be an ABq with α-O group



What kind of pattern is this? AB

(e) Show a structure for **R-12B**. If there is more than one possibility, circle your best choice.

8

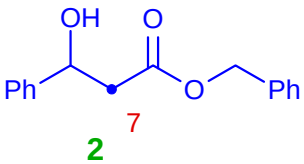


1

Base	1.20
α-OC(O)Alk	2.95
α-Ph	1.45
	5.60

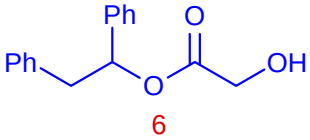
Obs: 5.07

17 other structures, including:

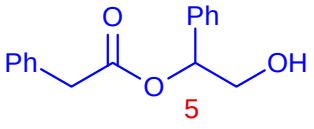


7

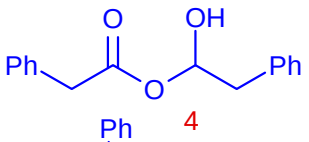
2



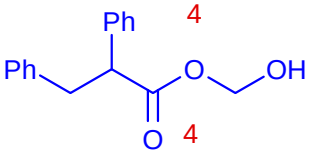
6



5



4 (nutty)



4 (nutty)

(f) Do a chemical shift calculation (from methane as model) of the carbon in your structure you have assigned the signal at δ 40.3. Show parameters you used.

4

1

Base	-2.1
α_{Ph}-n	23
α_C	9,1
β_{CO2R}-n	3
β_{OH}-iso	8
	41.0

2

Base	-2.1
α_{CO2R}-n	20
α_C	9,1
β_{Ph}-n	9
β_{OH}-iso	8
	44.0

Observed: 40.3