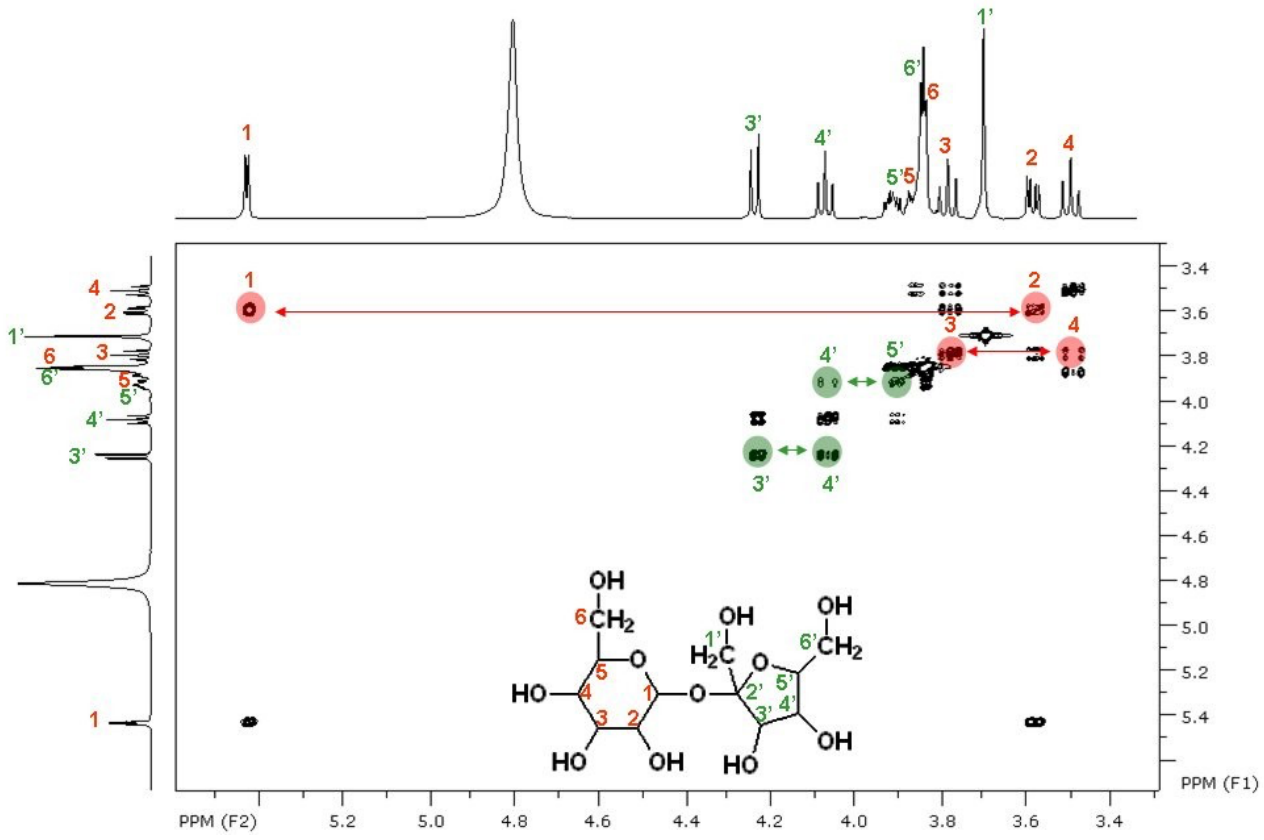
NMR SPECTROSCOPY



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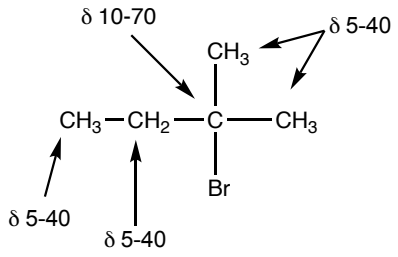
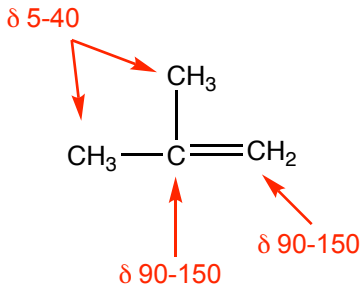
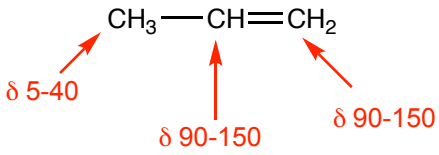
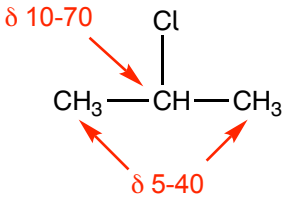
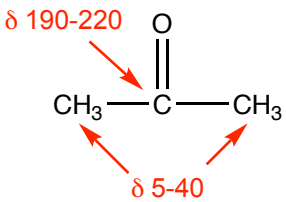
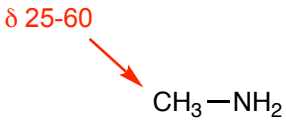
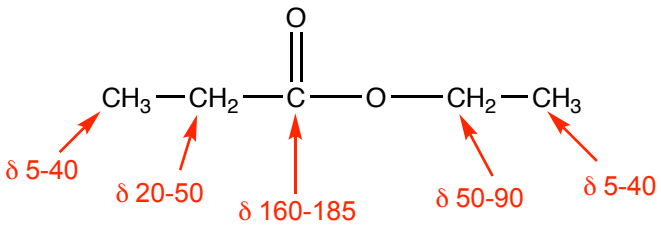
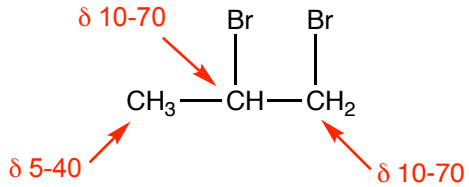
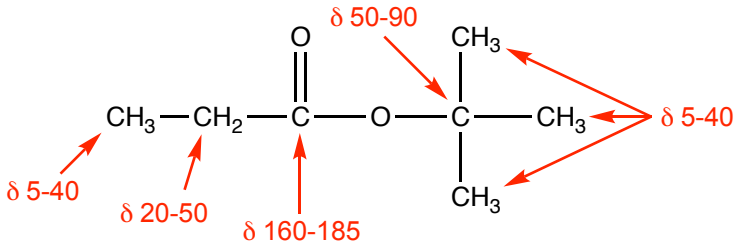
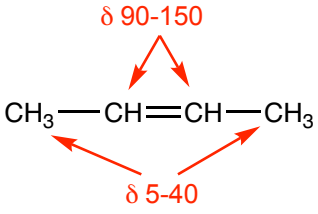
TASK 1 – Predicting ^{13}C NMR spectra

Compound	Structure and chemical shift (δ)	Number of signals
2-bromo-2-methylbutane		4
methylpropene		3
propene		3
2-chloropropane		2
propanone		2

Compound	Structure and chemical shift (δ)	Number of signals
methylamine		1
ethyl propanoate		5
1,2-dibromopropane		3
dimethylethyl propanoate		5
but-2-ene		2

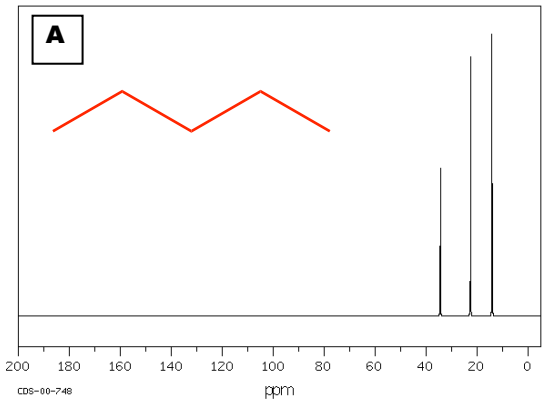
TASK 2 – Which ^{13}C NMR spectrum is which?

For each of the following compounds:

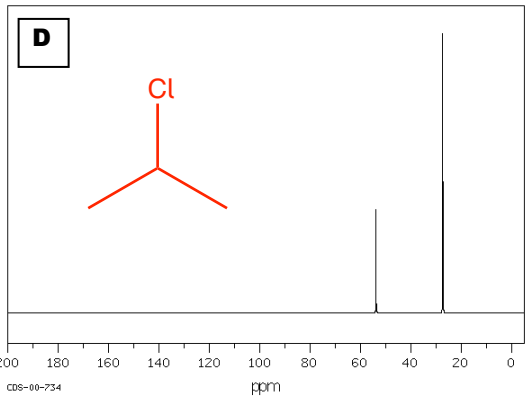
propanoic acid pentane 2-chlorpropane propanone 2,2-dichloropropane 2,3-dimethylbut-2-ene

Work out which spectrum belongs to which compound.

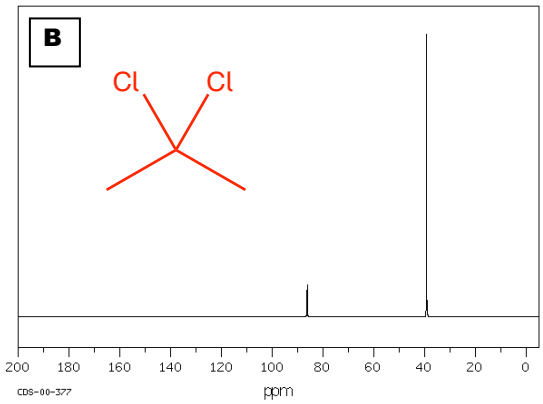
A



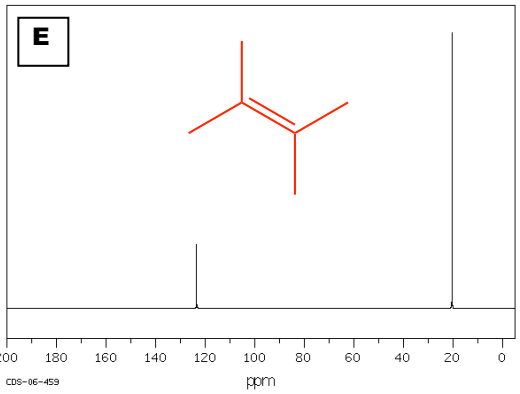
D



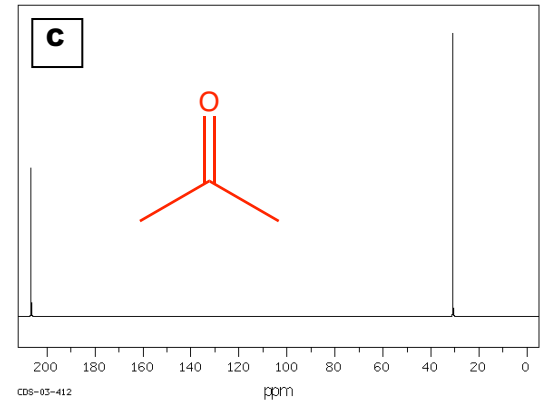
B



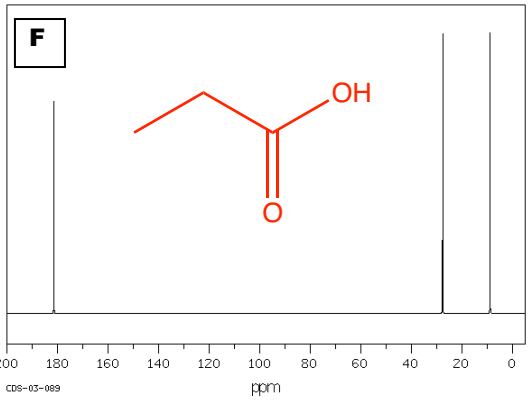
E



C

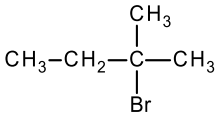
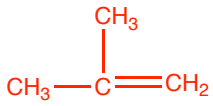
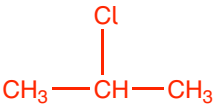
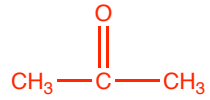
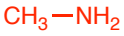
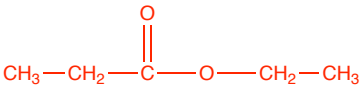
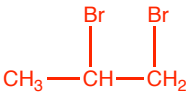
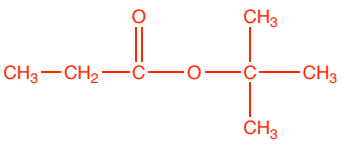
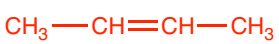


F



TASK 3a/b – Predicting ^{1}H NMR spectra 1

Complete the second, third and fourth columns in this table.

Compound	Structure	Number of signals	Relative intensity of signals	Splitting patterns of signals
2-bromo-2-methylbutane		3	3 : 2 : 6	t, q, s
methylpropene		2	6 : 2 (i.e. 3 : 1)	s, s
propene		3	3 : 1 : 2	d, m, d
2-chloropropane		2	6 : 1	d, m
propanone		1		s
methylamine		2	3 : 2	s, s
ethyl propanoate		4	3 : 2 : 2 : 3	t, q, q, t
1,2-dibromopropane		3	3 : 1 : 2	d, m, d
dimethylethyl propanoate		3	3 : 2 : 9	t, q, s
but-2-ene		2	6 : 2 (3 : 1)	d, q

TASK 4 – Finding the relative intensity of signals from a spectrum

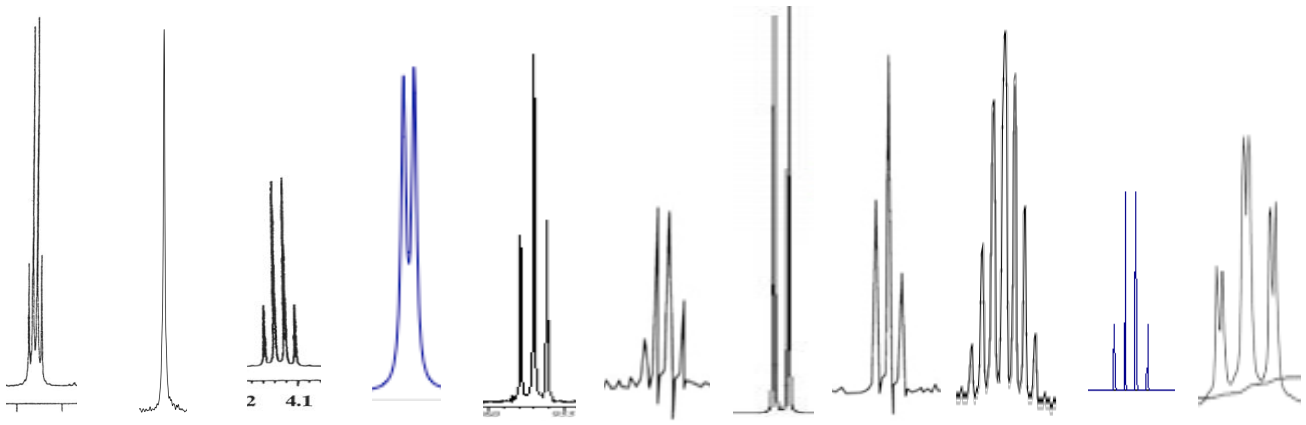
Spectrum A: 1 : 6 : 2 : 3

Spectrum B: 2 : 2 : 3 : 3

Spectrum C: 1 : 2

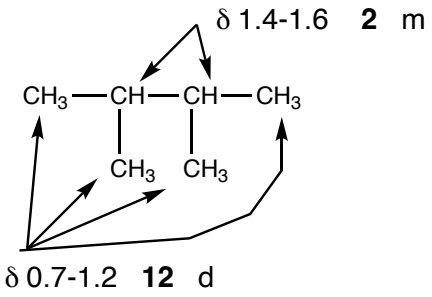
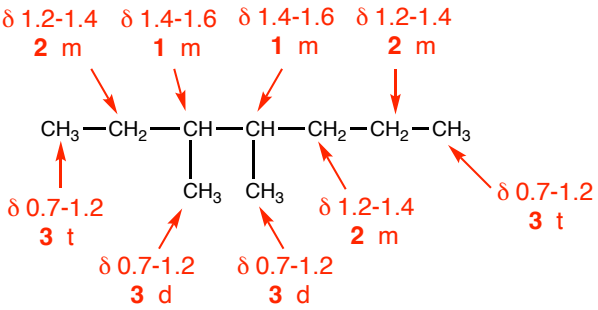
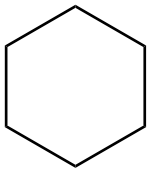
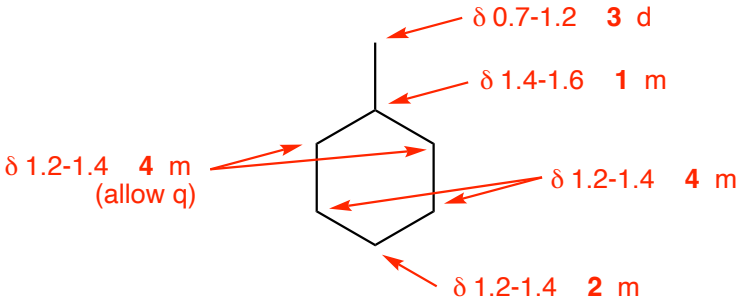
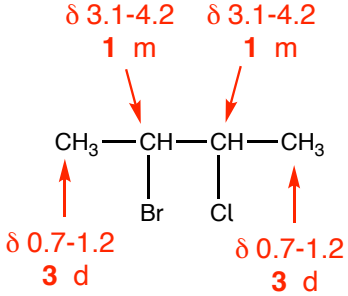
Spectrum D: 2 : 3

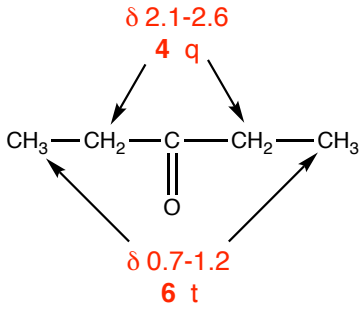
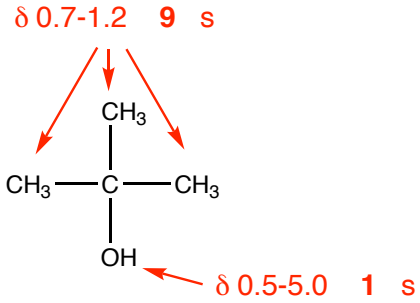
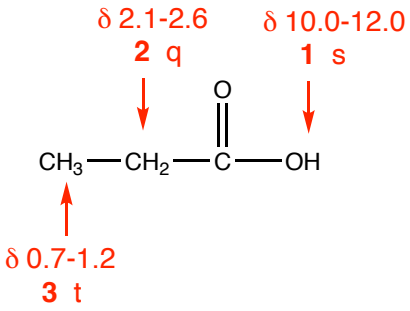
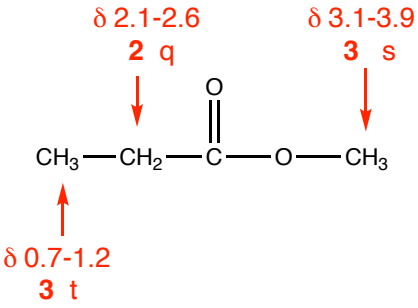
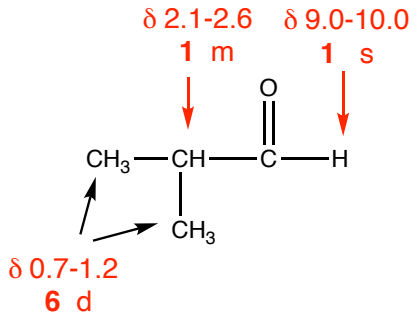
TASK 5 – Identifying splitting patterns



q s q d t q d t m q m

TASK 6 – Predicting ^{1}H NMR spectra

Compound	Structure, δ, relative intensity & splitting	Number of signals
2,3-dimethylbutane		2
3,4-dimethylheptane		9
cyclohexane	 one signal δ 1.2-1.4 s	1
methylcyclohexane		5
2-bromo-3-chlorobutane		4

Compound	Structure, δ, relative intensity & splitting	Number of signals
pentan-3-one		2
2-methylpropan-2-ol		2
propanoic acid		3
methyl propanoate		3
methylpropanal		3

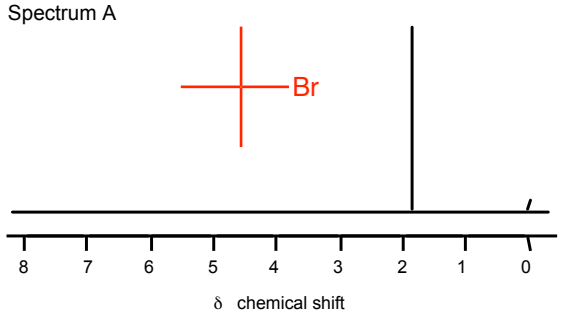
TASK 7 – Which ^{1}H NMR spectrum is which?

For each of the following compounds:

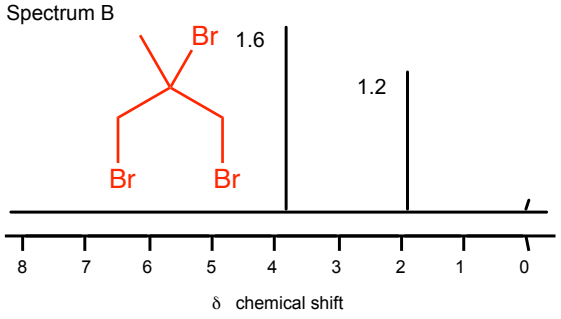
CH_3CH_2I $(CH_3)_3CBr$ CH_3COCH_2OH $(CH_3)_3COH$ $CH_2ClCHCl_2$ $(CH_2Br)_2CBrCH_3$ $(CH_3)_2CBrCH_2Br$

Work out which spectrum belongs to which compound.

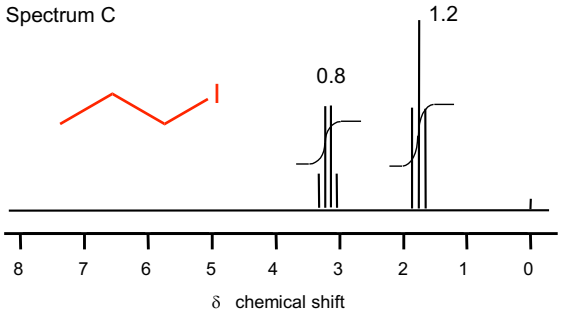
Spectrum A



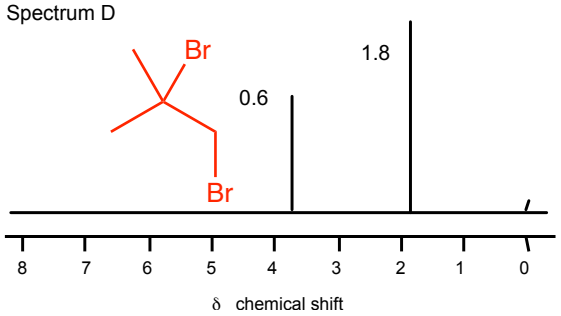
Spectrum B



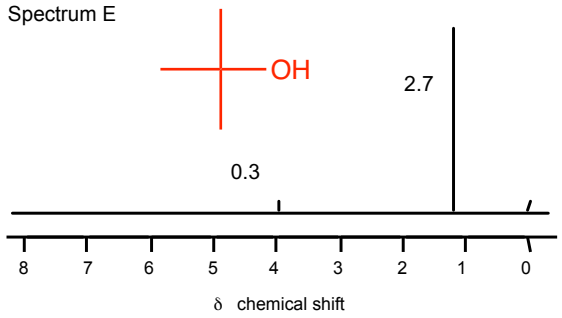
Spectrum C



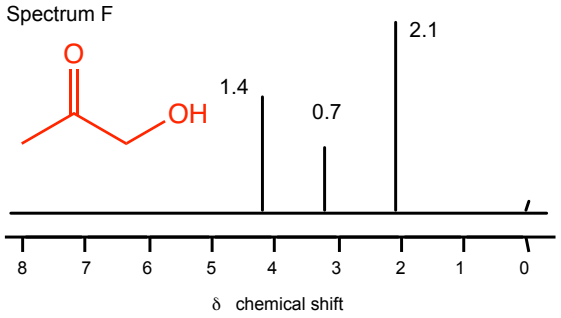
Spectrum D



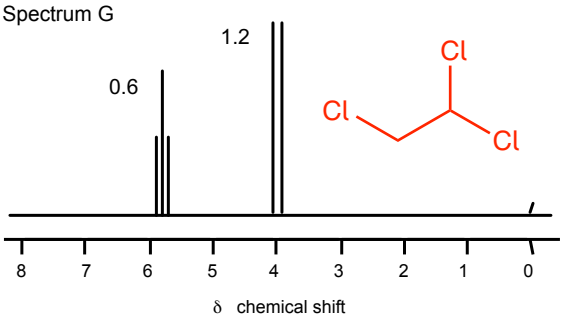
Spectrum E



Spectrum F



Spectrum G



TASK 8 – Identifying compounds

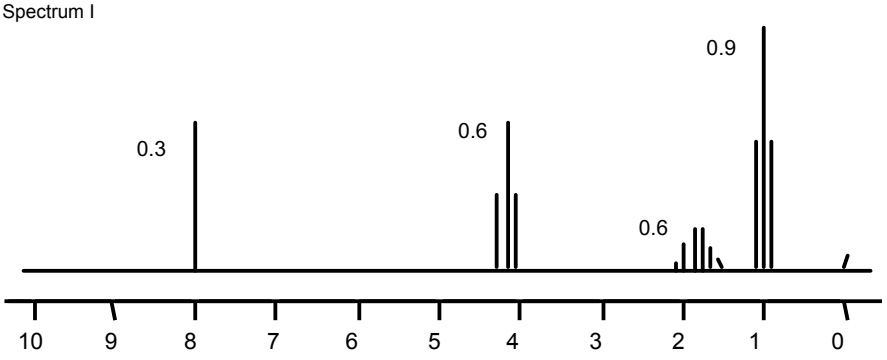
The ^1H NMR spectra of three isomers of $C_4H_8O_2$ are shown.

a) Draw the structural formulae of all the isomers of $C_4H_8O_2$ that are carboxylic acids or esters.

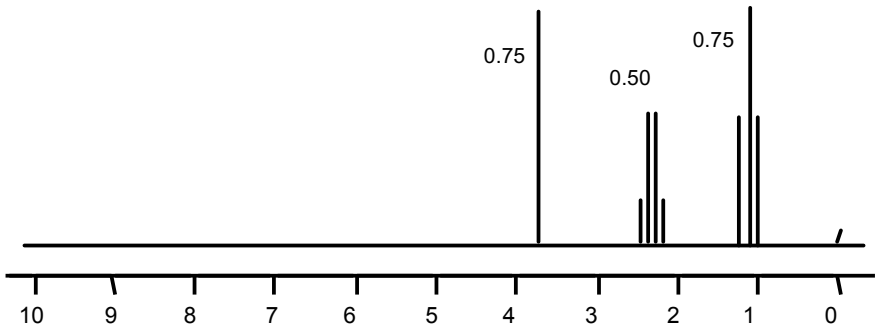
b) Indicate the number of signals, and relative intensity and multiplicity of each signal for each isomer.

c) Deduce which spectrum belongs to which isomer.

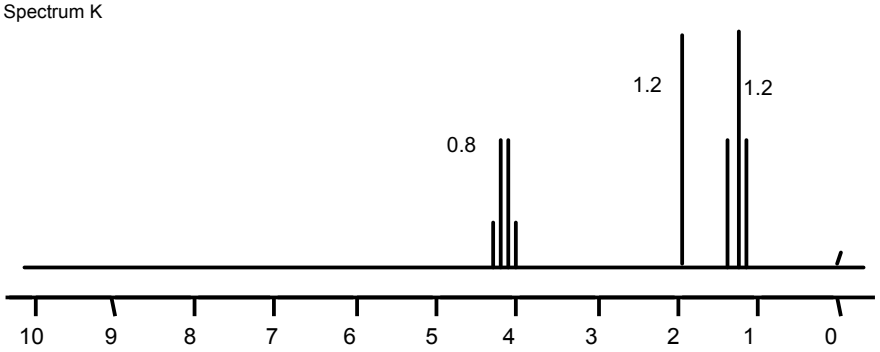
Spectrum I

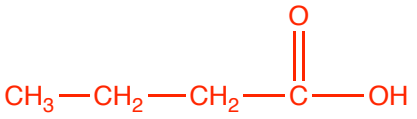


Spectrum J



Spectrum K

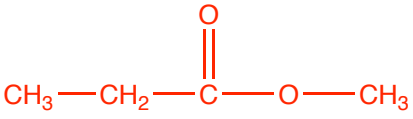




3 2 2 1

t m t s

δ 2.1-2.6 δ 10-12

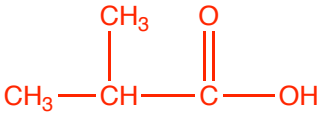


J

3 2 3

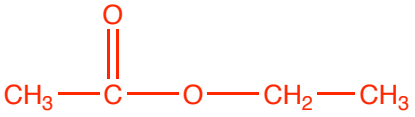
t q s

δ 3.1-3.9



6 1 1

d m s

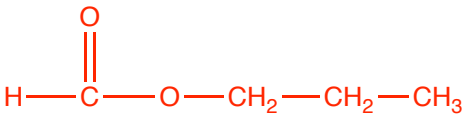


K

3 2 3

s q s

δ 2.1-2.6

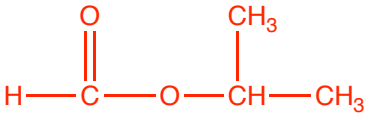


I

1 2 2 3

s t m t

δ 9-10 δ 3.1-3.9

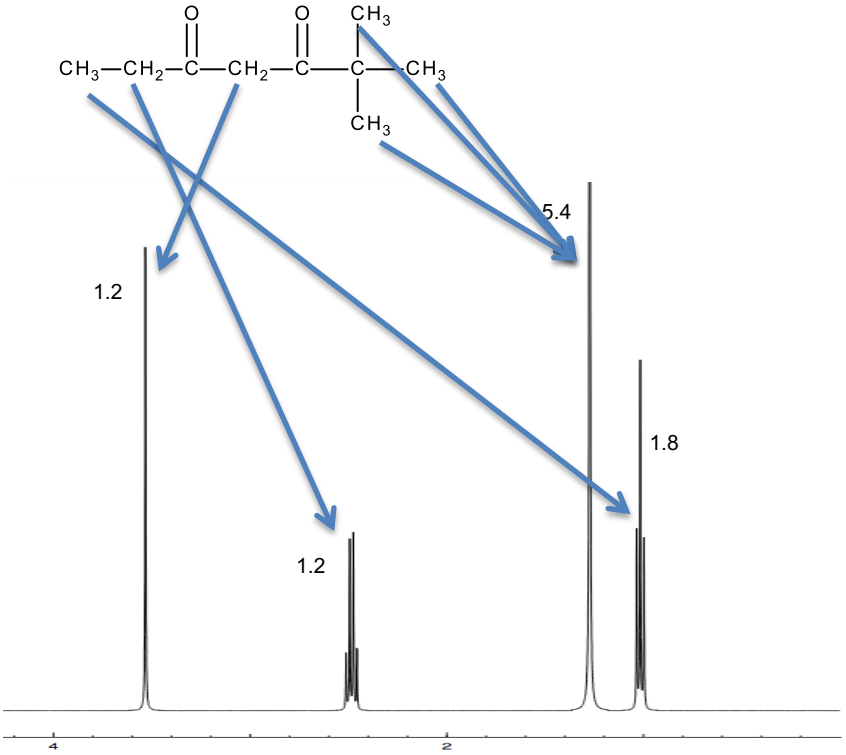


1 1 6

s m d

TASK 9 – Identifying compounds using ^{1}H NMR

1



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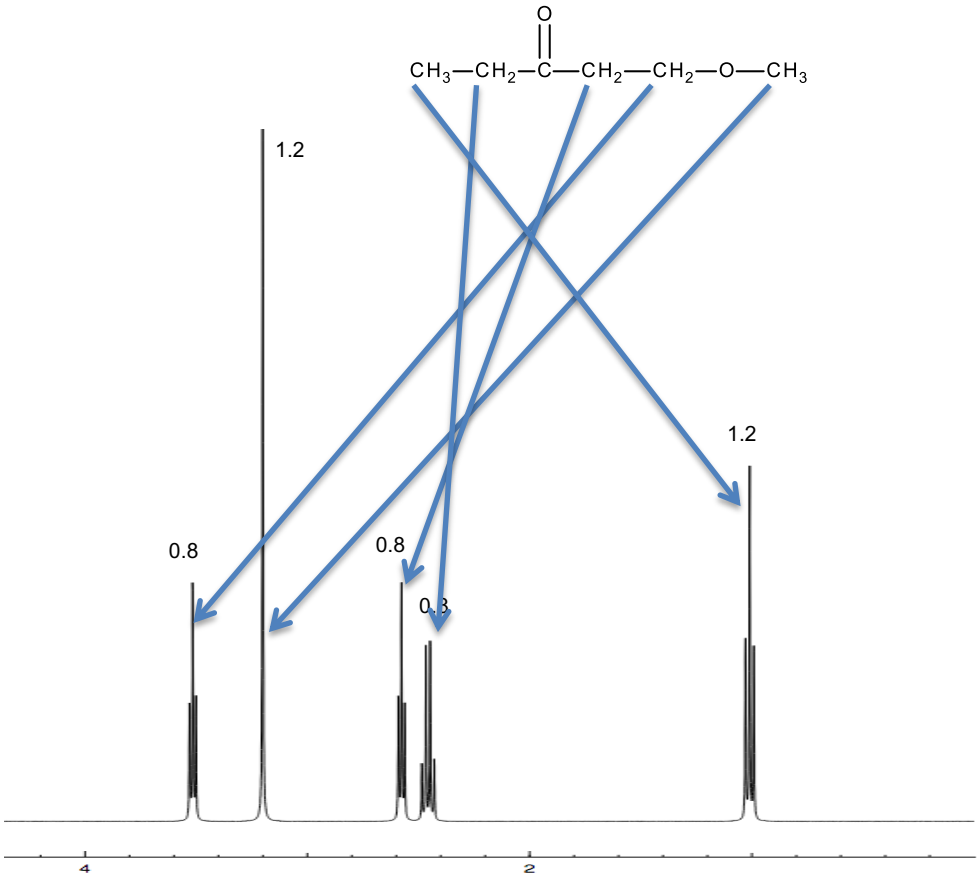

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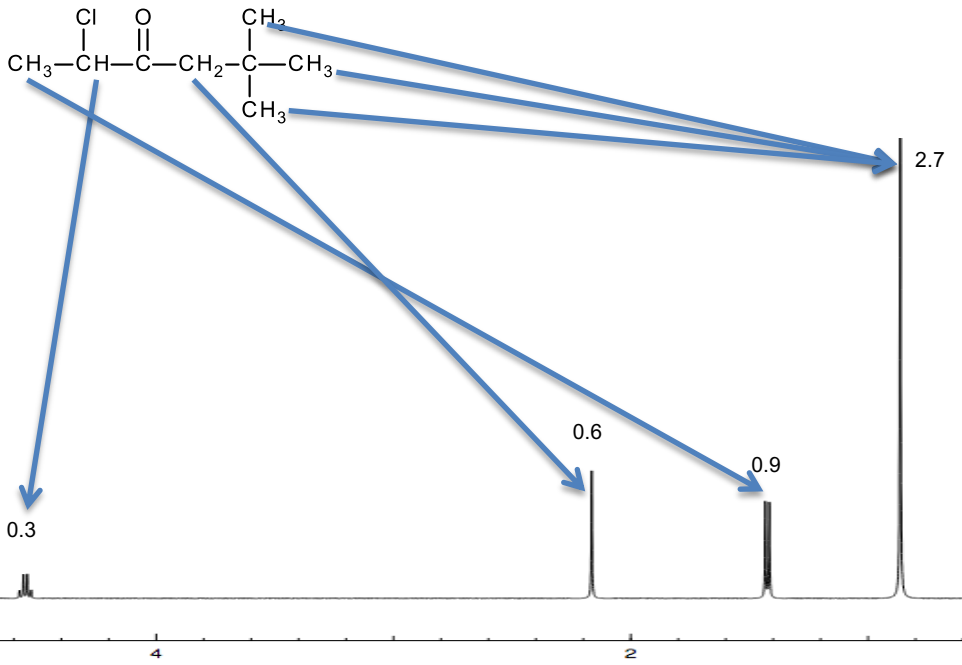

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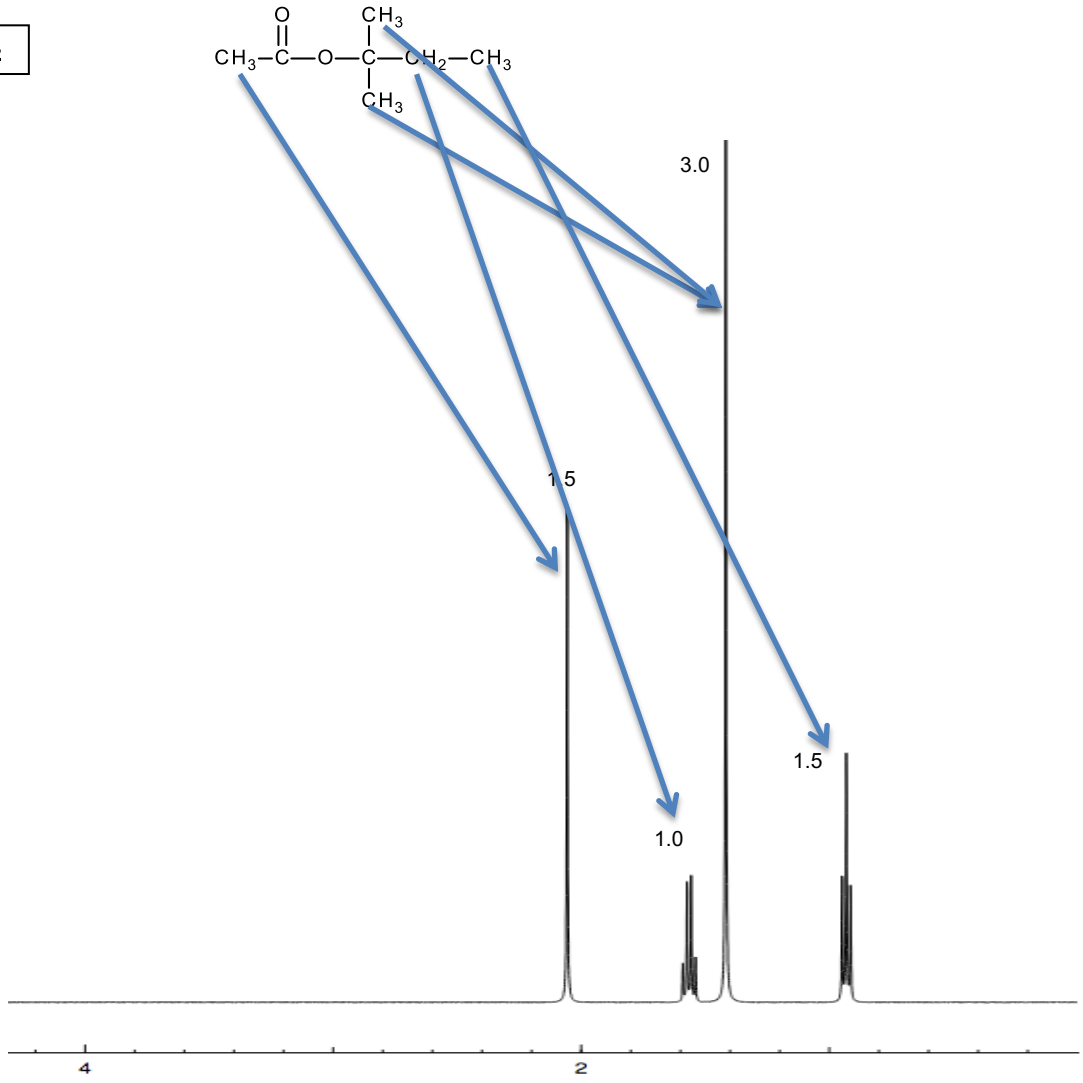
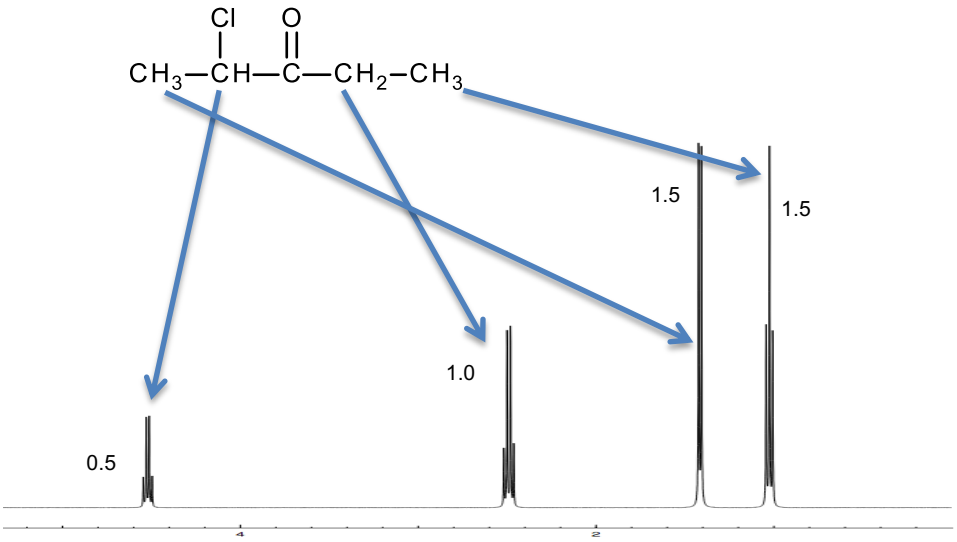
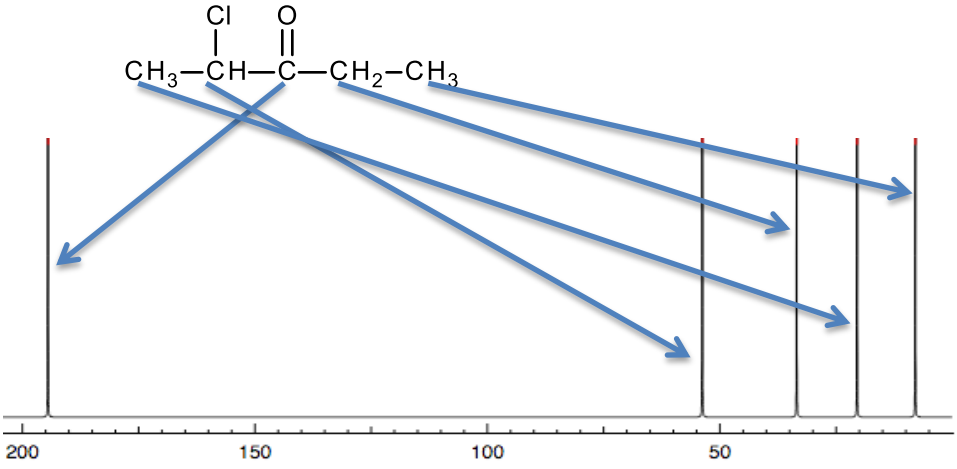


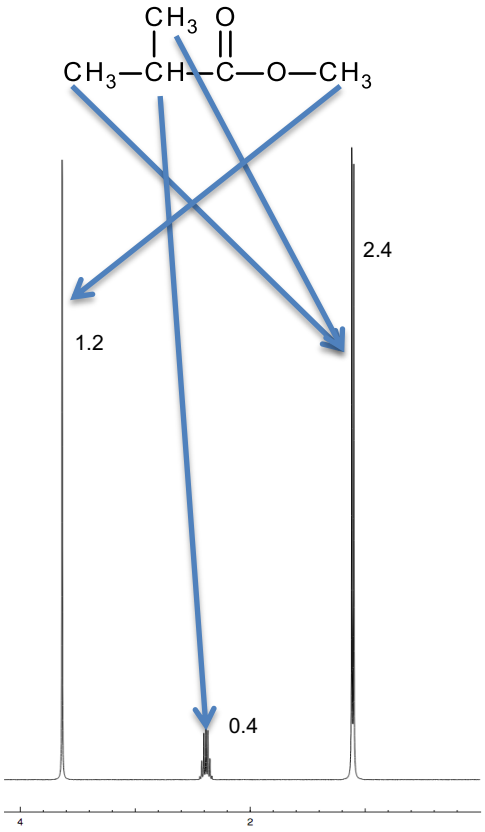
TASK 10 – Using ^{1}H and ^{13}C NMR together to identify compounds

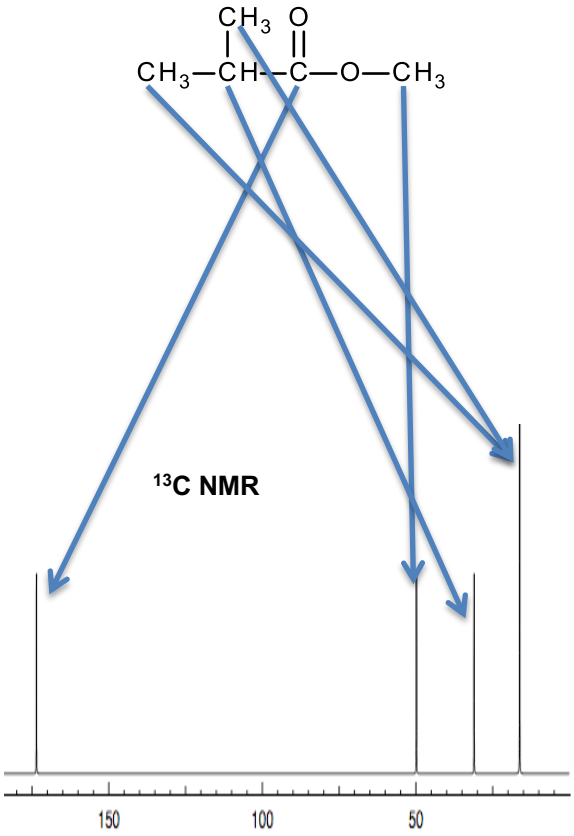
1 The ^{1}H and ^{13}C NMR spectra of C_5H_9OCl are shown. Deduce the structure of the compound and then explain each signal.



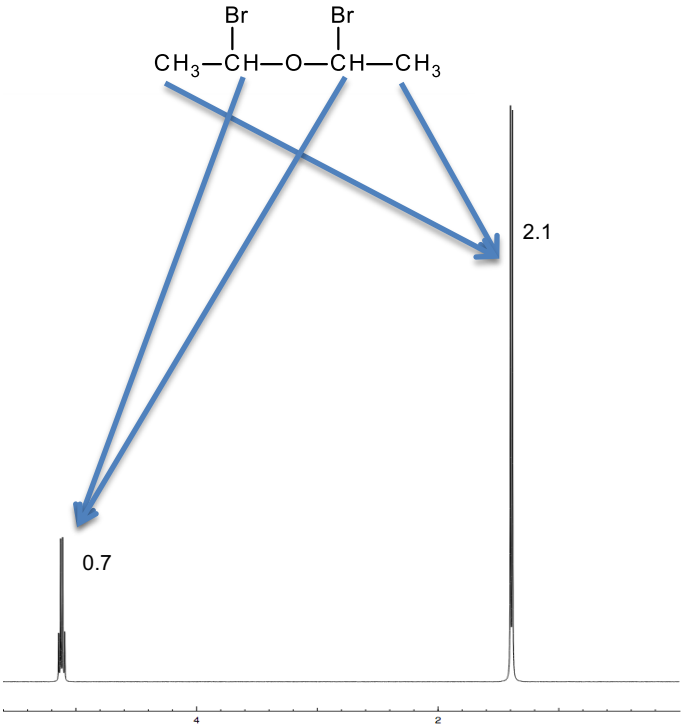


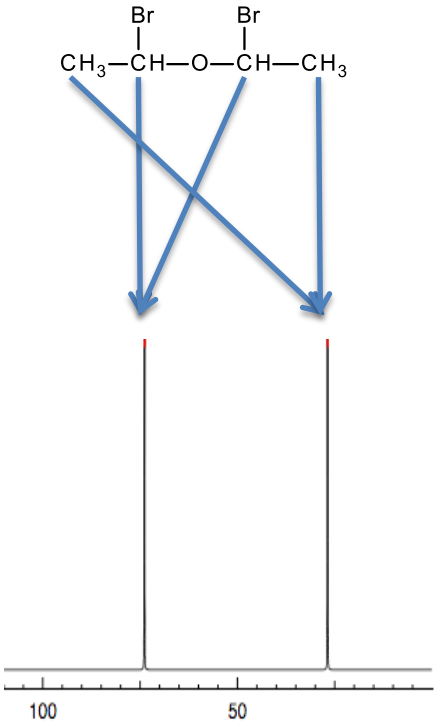
2 The ^{1}H and ^{13}C NMR spectra of $C_5H_{10}O_2$ are shown. Deduce the structure of the compound and then explain each signal.



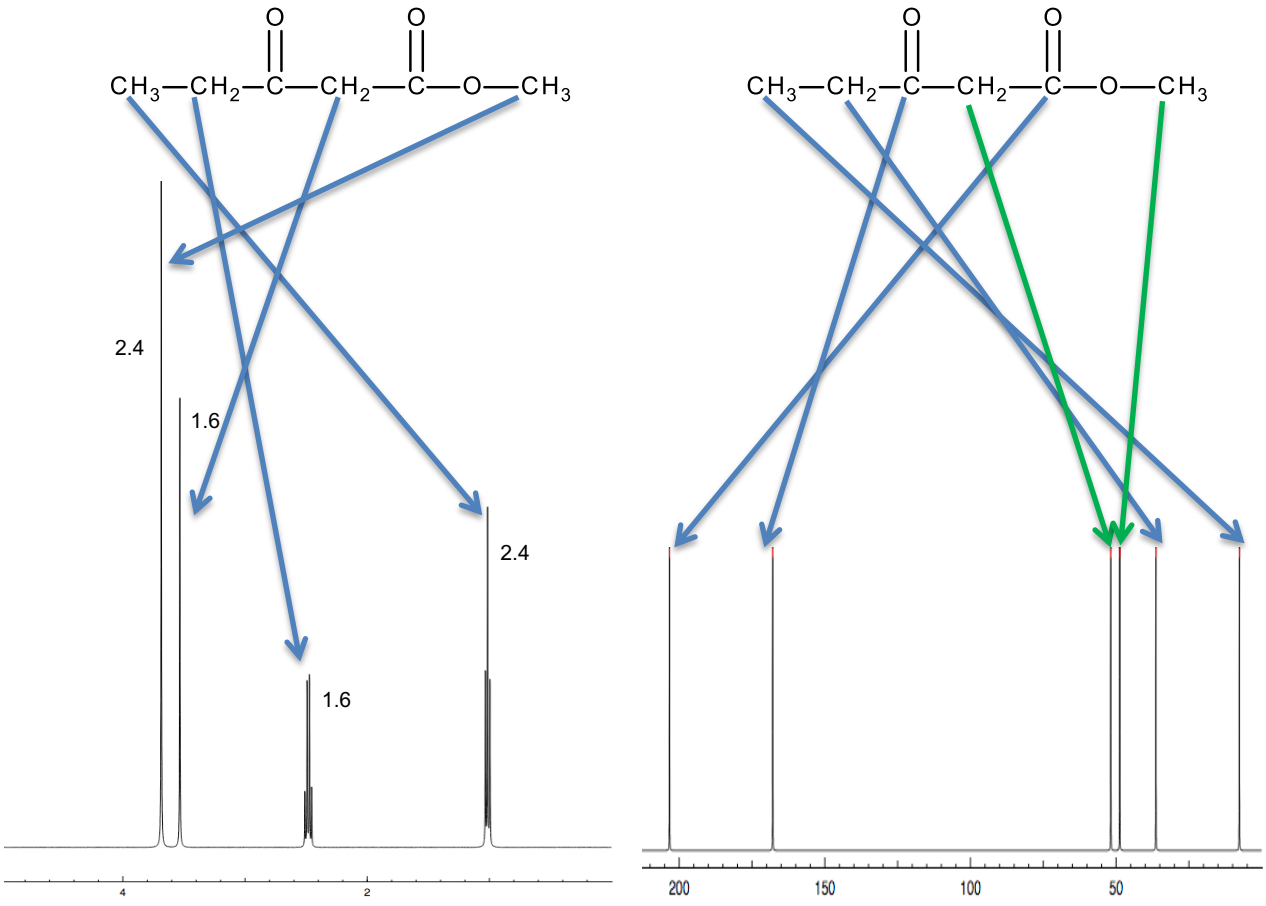


3 The ^{1}H and ^{13}C NMR spectra of $C_4H_8OBr_2$ are shown. Deduce the structure of the compound and then explain each signal.





4 The ^{1}H and ^{13}C NMR spectra of $C_6H_{10}O_3$ are shown. Deduce the structure of the compound and then explain each signal.



lack of certainty as to which signal is which