NMR SPECTROSCOPY

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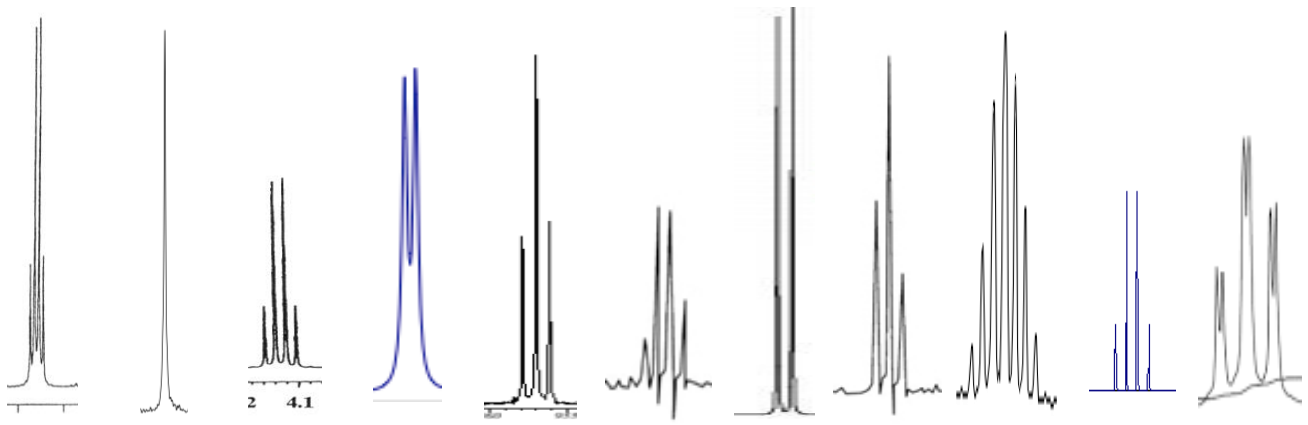
TASK 2 – Finding the relative intensity of signals from a spectrum

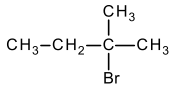
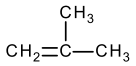
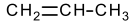
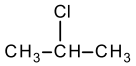
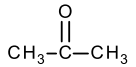
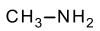
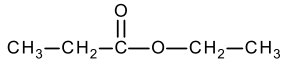
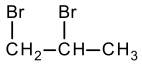
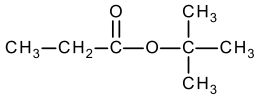
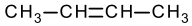
Spectrum A: 1 : 6 : 2 : 3
Spectrum B: 2 : 2 : 3 : 3
Spectrum C: 1 : 2
Spectrum D: 2 : 3

TASK 3 – Identifying splitting patterns

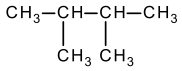
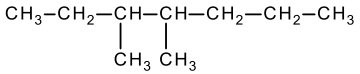
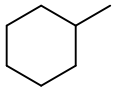
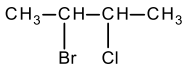
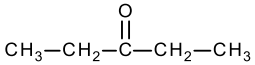
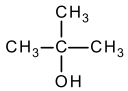
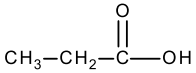
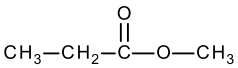
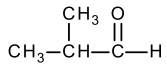


q s q d t q d t m q m

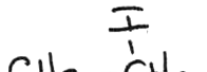
TASK 1 – Predicting ^{1}H NMR spectra

Compound	Structure	Number of signals	Relative intensity of signals	Splitting patterns of signals	Position of signals
2-bromo-2-methylbutane		3	3 : 2 : 6	t, q, s	δ 0.7-1.2 (3, t) δ 1.2-1.4 (2, q) δ 0.7-1.2 (6, s)
methylpropene		2	3 : 1	s, s	δ 0.7-1.2 (3, s) δ 4.5-6.0 (1, s)
propene		3	2 : 1 : 3	d, m, d	δ 0.7-1.2 (3, d) δ 4.5-6.0 (1, m) δ 4.5-6.0 (2, d)
2-chloropropane		2	6 : 1	d, m	δ 0.7-1.2 (6, d) δ 3.1-3.9 (1, m)
propanone		1		s	δ 2.1-2.6 (s)
methylamine		2	3 : 2	t, q	δ 0.7-1.2 (3, t) δ 1.0-4.5 (2, q)
ethyl propanoate		4	3 : 2 : 2 : 3	t, q, q, t	δ 0.7-1.2 (3, t), δ 0.7-1.2 (3, t) δ 2.1-2.6 (2, q), δ 3.7-4.1 (2, q)
1,2-dibromopropane		3	2 : 1 : 3	d, m, d	δ 3.1-4.2 (2, d) δ 3.1-4.2 (1, m) δ 0.7-1.2 (3, d)
dimethylethyl propanoate		3	3 : 2 : 9	t, q, s	δ 0.7-1.2 (3, t) δ 2.1-2.6 (2, q) δ 0.7-1.2 (9, s)
but-2-ene		2	3 : 1	d, q	δ 0.7-1.2 (3, d) δ 4.5-6.0 (1, q)

TASK 4 – Predicting ^{1}H NMR spectra

Compound	Structure	Number of signals	Relative intensity of signals	Splitting patterns of signals	Position of signals
2,3-dimethylbutane		2	6 : 1	d, m	δ 0.7-1.2 (6, d) δ 1.4-1.6 (1, m)
3,4-dimethylheptane		9	3 : 2 : 1 : 3 : 1 : 3 : 2 : 2 : 3	t, m, m, d, m, d, q, m, t	δ 0.7-1.2 (3, t), δ 1.2-1.4 (2, m), δ 1.4-1.6 (1, m), δ 0.7-1.2 (3, d), δ 1.4-1.6 (1, m), δ 0.7-1.2 (3, d), δ 1.2-1.4 (2, q), δ 1.2-1.4 (2, m), δ 0.7-1.2 (3, t)
cyclohexane		1		s	δ 1.2-1.4 (2, s)
methylcyclohexane		5	3 : 1 : 4 : 4 : 2	d, m, q, m, m	δ 0.7-1.2 (3, d), δ 1.4-1.6 (1, m), δ 1.2-1.4 (4, q), δ 1.2-1.4 (4, m), δ 1.2-1.4 (2, m)
2-bromo-3-chlorobutane		4	3 : 1 : 1 : 3	d, m, m, d	δ 0.7-1.2 (3, d), δ 3.1-4.2 (1, m) δ 3.1-4.2 (1, m), δ 0.7-1.2 (3, d)
pentan-3-one		2	3 : 2	t, q	δ 0.7-1.2 (3, t) δ 2.1-2.6 (2, q)
2-methylpropan-2-ol		2	9 : 1	s, s	δ 0.7-1.2 (9, s) δ 0.5-5.0 (1, s)
propanoic acid		3	3 : 2 : 1	t, q, s	δ 0.7-1.2 (3, t) δ 2.1-2.6 (2, q) δ 10.0-12.0 (1, s)
methyl propanoate		3	3 : 2 : 3	t, q, s	δ 0.7-1.2 (3, t) δ 2.1-2.6 (2, q) δ 3.7-4.1 (3, s)
methylpropanal		3	6 : 1 : 1	d, m, d	δ 0.7-1.2 (6, d) δ 2.1-2.6 (1, m) δ 9.0-10.0 (1, d)

TASK 5 – Which ^{1}H NMR spectrum is which?

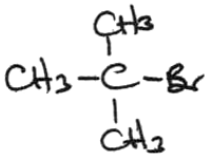


(2)

3 : 2

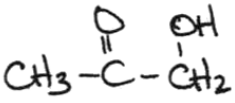
t q

(C)



(1)

(A)

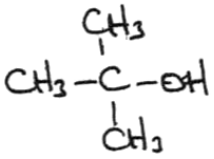


(3)

3 : 2 : 1

s s s

(F)

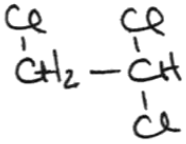


(2)

9 : 1

s s

(E)

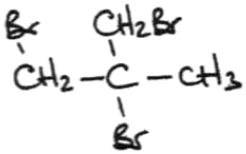


(2)

2 : 1

d t

(G)

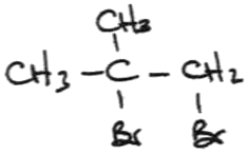


(2)

4 : 3

s s

(B)



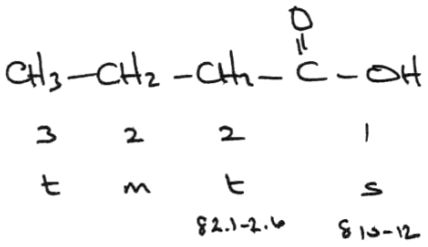
(2)

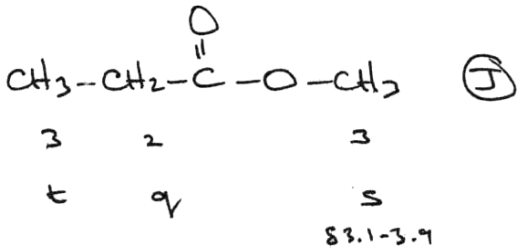
3 : 1

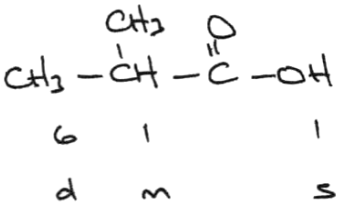
s s

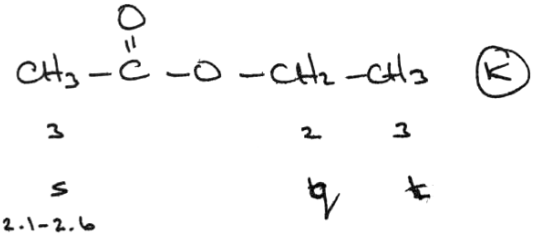
(D)

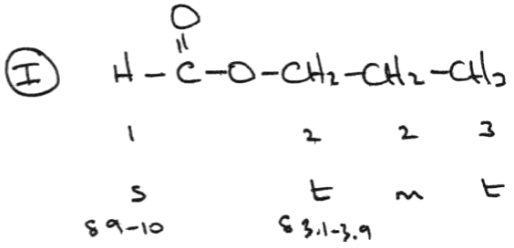
TASK 6 – Identifying compounds

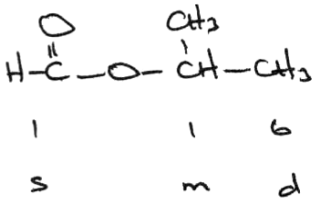






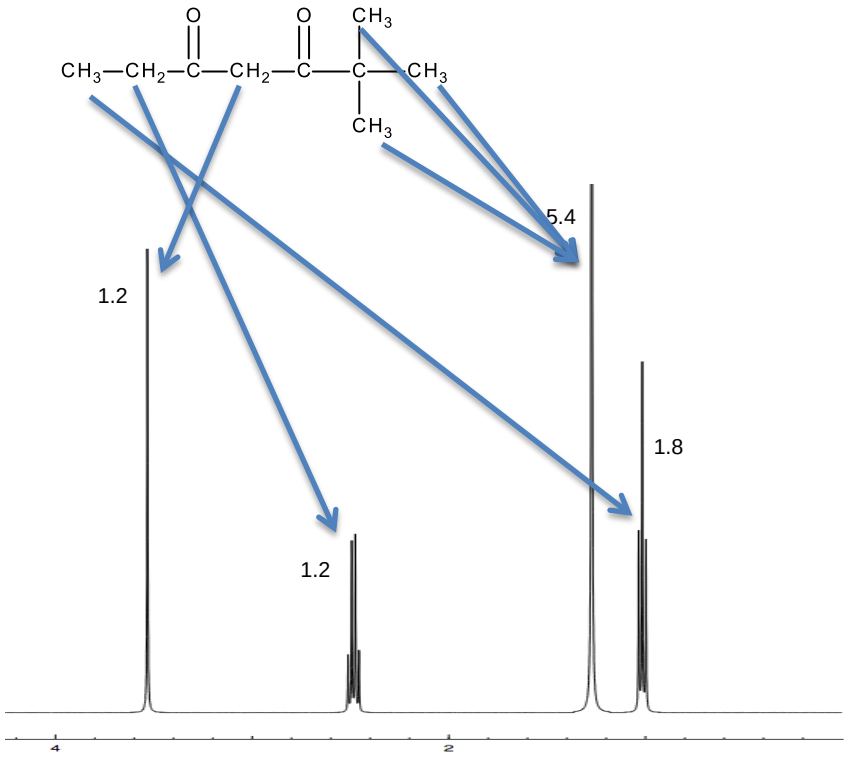




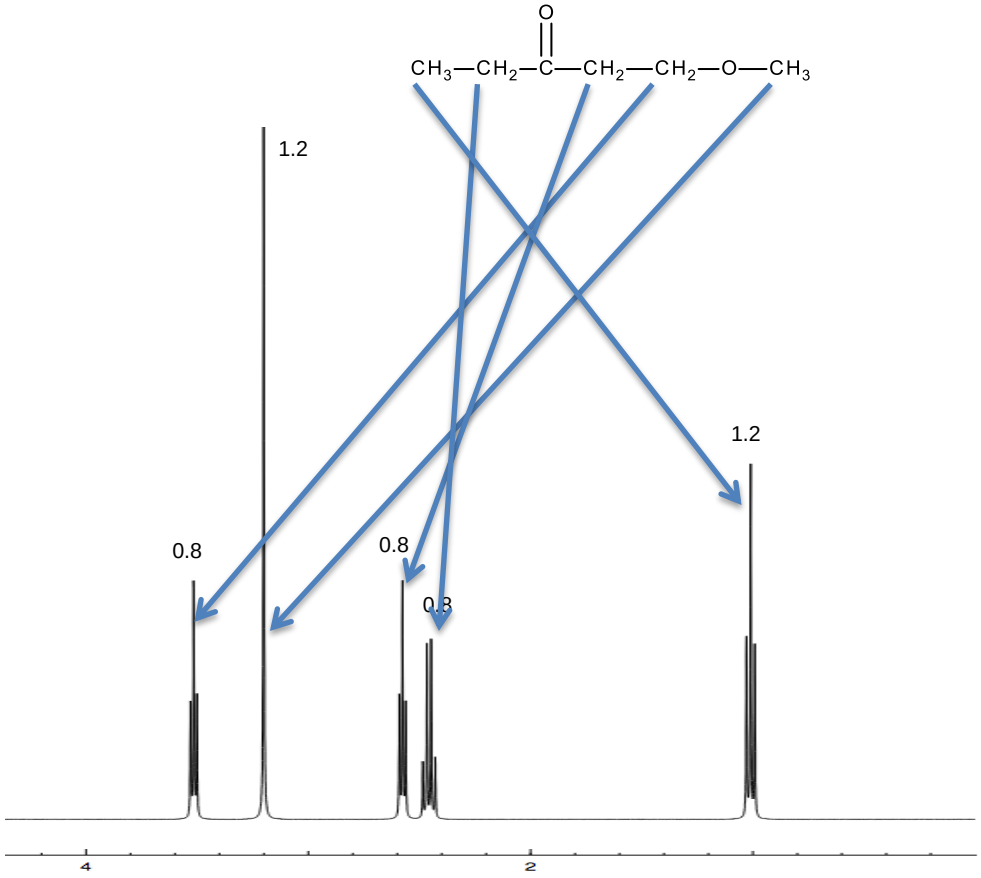


TASK 7 – Identifying compounds using ^{1}H NMR

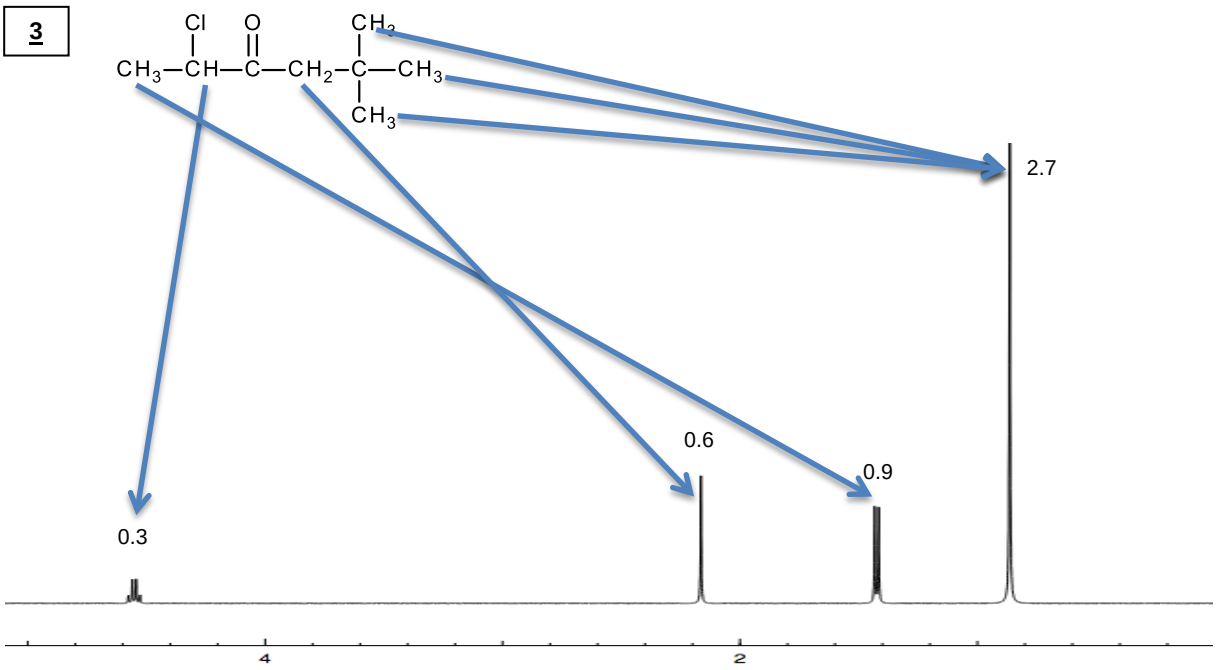
1



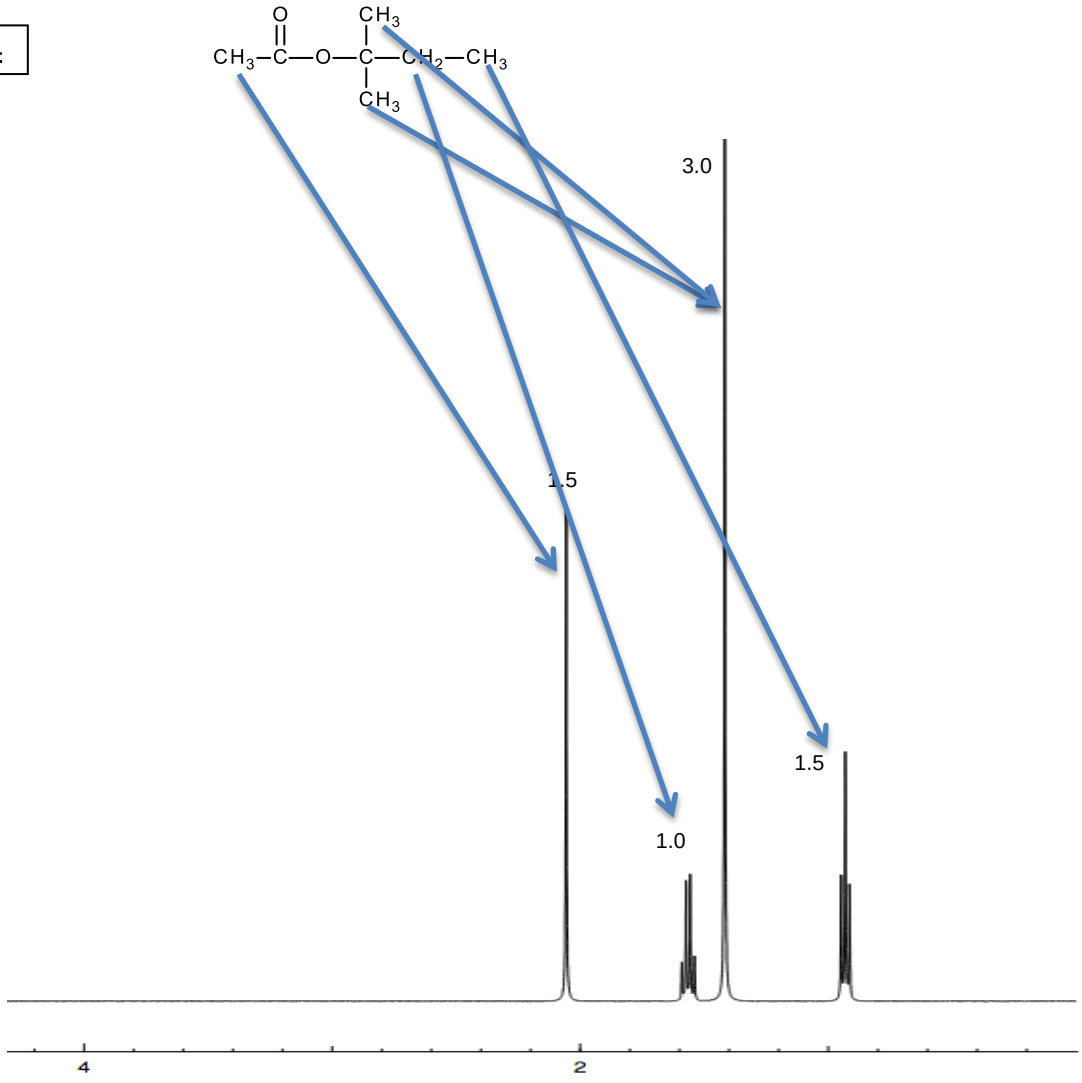
2



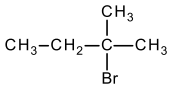
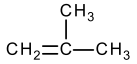
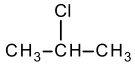
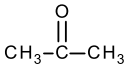
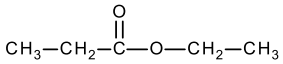
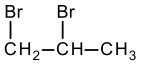
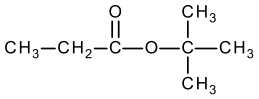
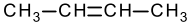
3


Cl
O
CH3
CH3—CH—C—CH2—C—CH3
CH3
2.7
0.6
0.9
0.3
4
2

4

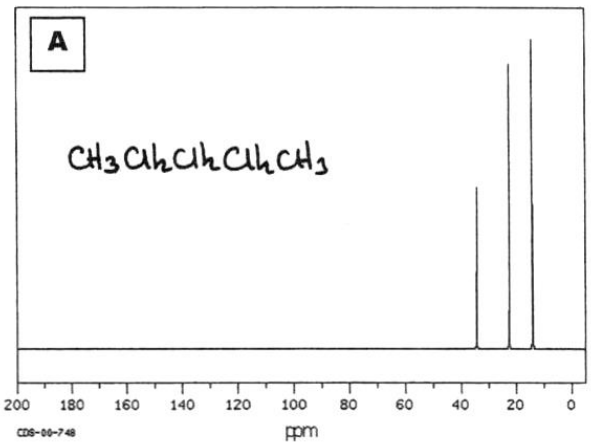

O
CH3
CH3—C—O—C—CH2—CH3
CH3
3.0
1.5
1.5
1.0
4
2

TASK 8 – Predicting ^{13}C NMR spectra

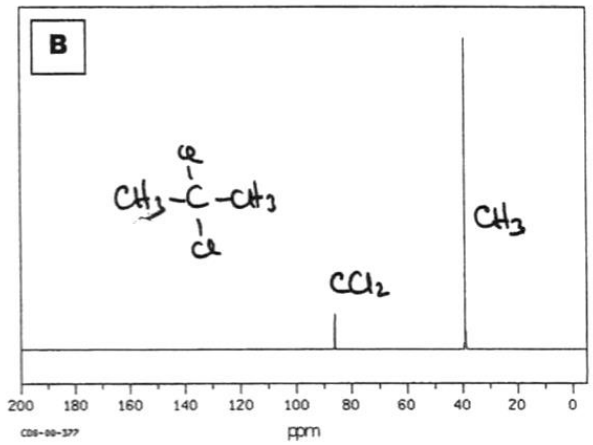
Compound	Structure	Number of signals	Position of signals
2-bromo-2-methylbutane		4	δ 5-40 (**C**H_3CH_2), δ 5-40 (CH_3**C**H_2), δ 10-70 (CBr), δ 5-40 (($$C$$$H_3)_2$CBr)
methylpropene		3	δ 90-150 (**C**H_2), δ 90-150 (**C**), δ 5-40 (($$C$$$H_3)_2$)
propene		3	δ 90-150 (**C**H_2), δ 90-150 (**C**), δ 5-40 (**C**H_3)
2-chloropropane		2	δ 5-40 (**C**H_3), δ 10-70 (**C**HCl)
propanone		2	δ 20-50 (**C**H_3), δ 190-220 (**C**O)
methylamine		1	δ 25-60 (**C**H_3)
ethyl propanoate		5	δ 5-40 (**C**H_3CH_2CO), δ 20-50 (**C**H_2CO), δ 160-185 (CO), δ 50-90 (O**C**H_2), δ 5-40 (OCH_2**C**H_3)
1,2-dibromopropane		3	δ 10-70 (**C**H_2Br), δ 10-70 (**C**HBr), δ 5-40 (**C**H_3)
dimethylethyl propanoate		5	δ 5-40 (**C**H_3CH_2CO), δ 20-50 (**C**H_2CO), δ 160-185 (CO), δ 50-90 (O**C**), δ 5-40 (OC**C**H_3)
but-2-ene		2	δ 5-40 (**C**H_3), δ 90-150 (**C**H)

TASK 9 – Which ^{13}C NMR spectrum is which?

A



B



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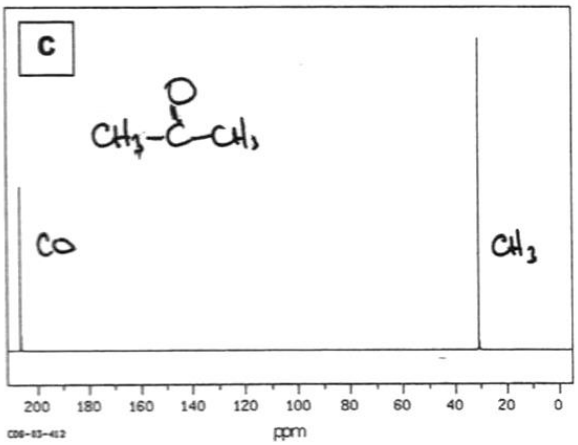

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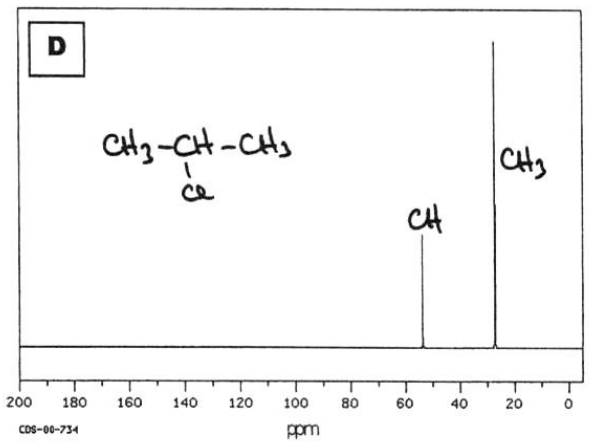

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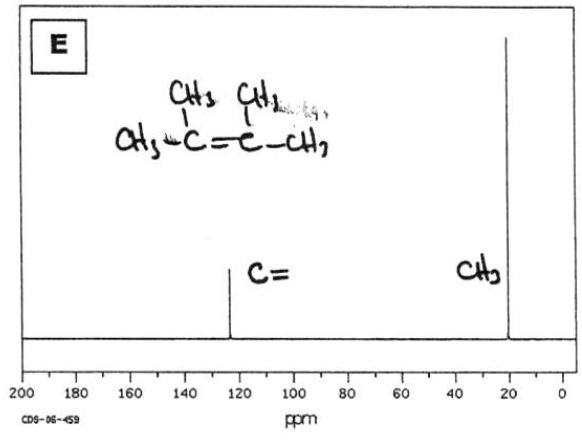

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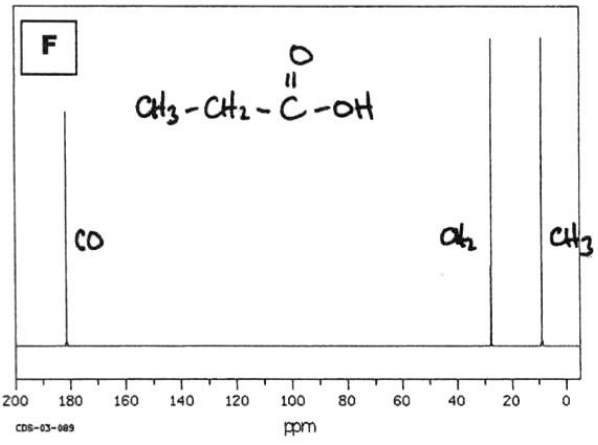
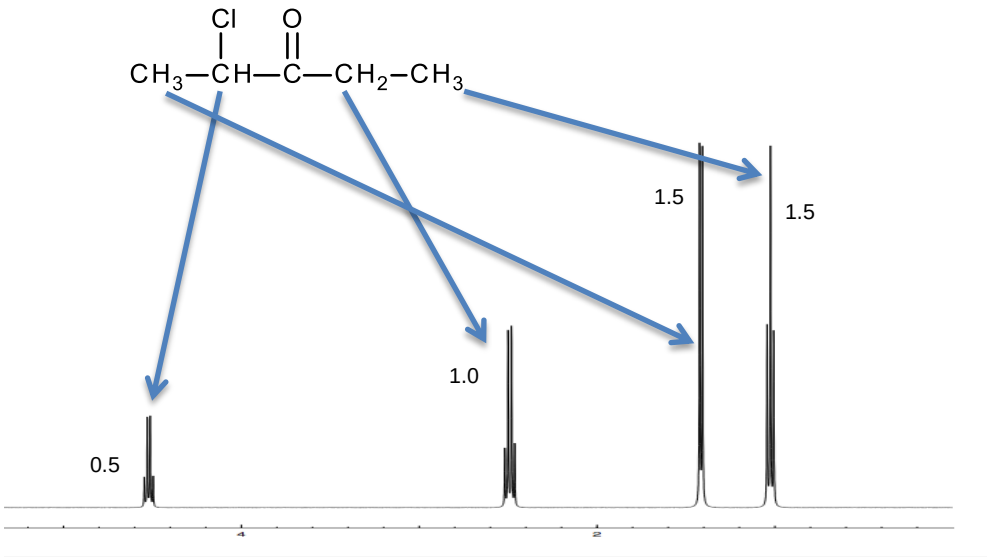
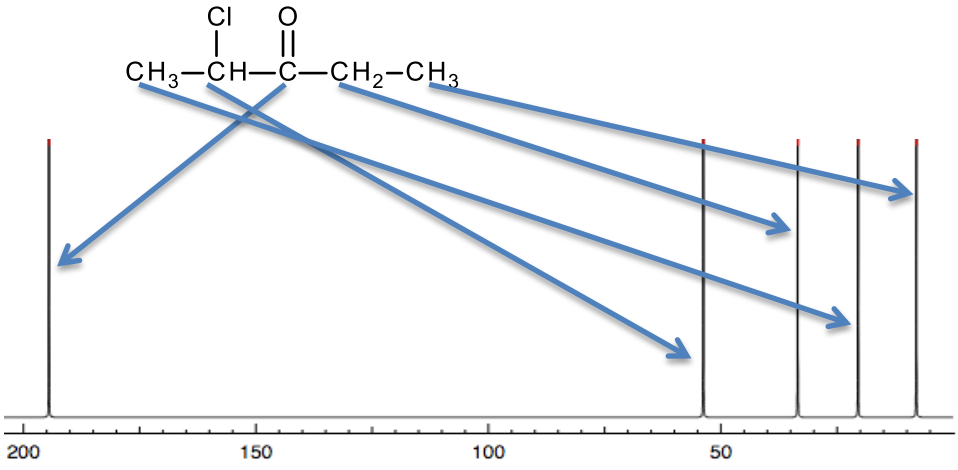


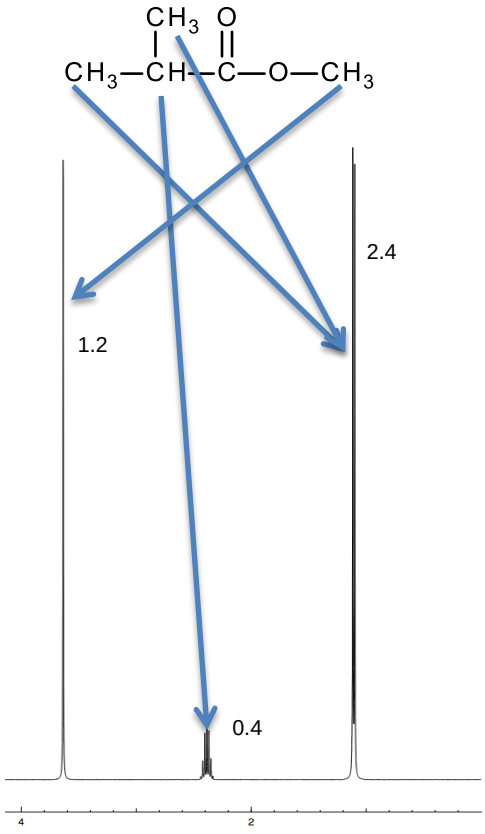
TASK 10 – Using ^{1}H and ^{13}C NMR together to identify compounds

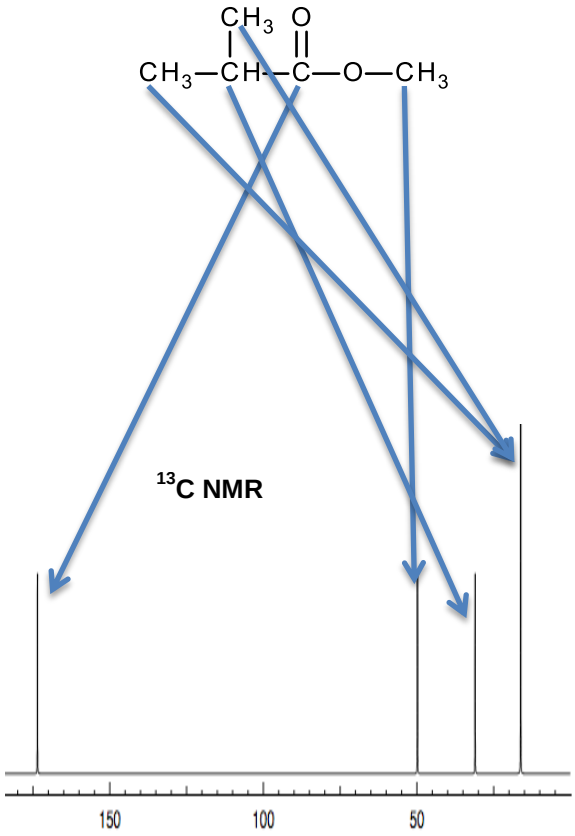
1 The ^{1}H and ^{13}C NMR spectra of C_5H_9OCl are shown. Deduce the structure of the compound and then explain each signal.



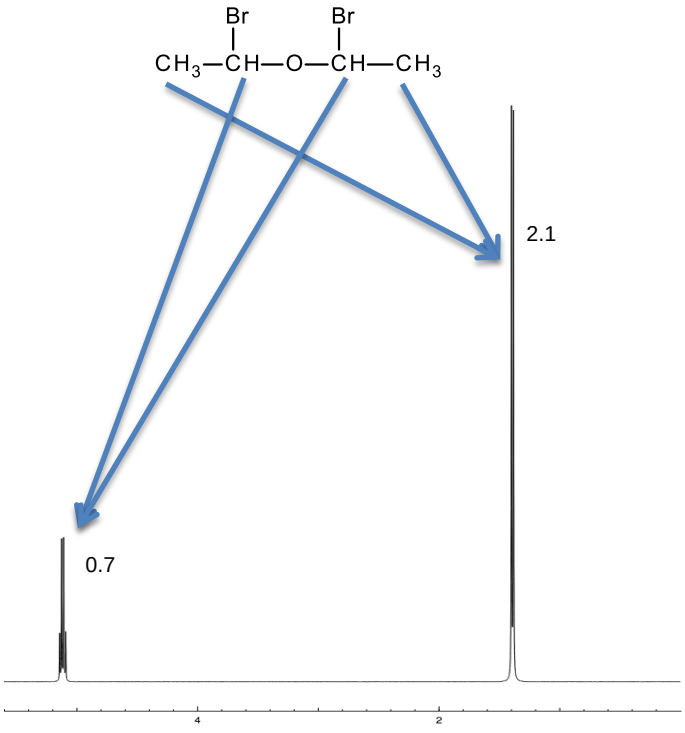


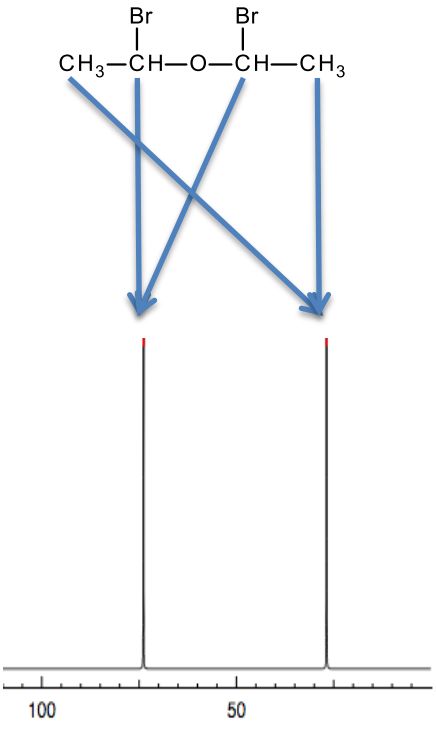
2 The ^{1}H and ^{13}C NMR spectra of $C_5H_{10}O_2$ are shown. Deduce the structure of the compound and then explain each signal.



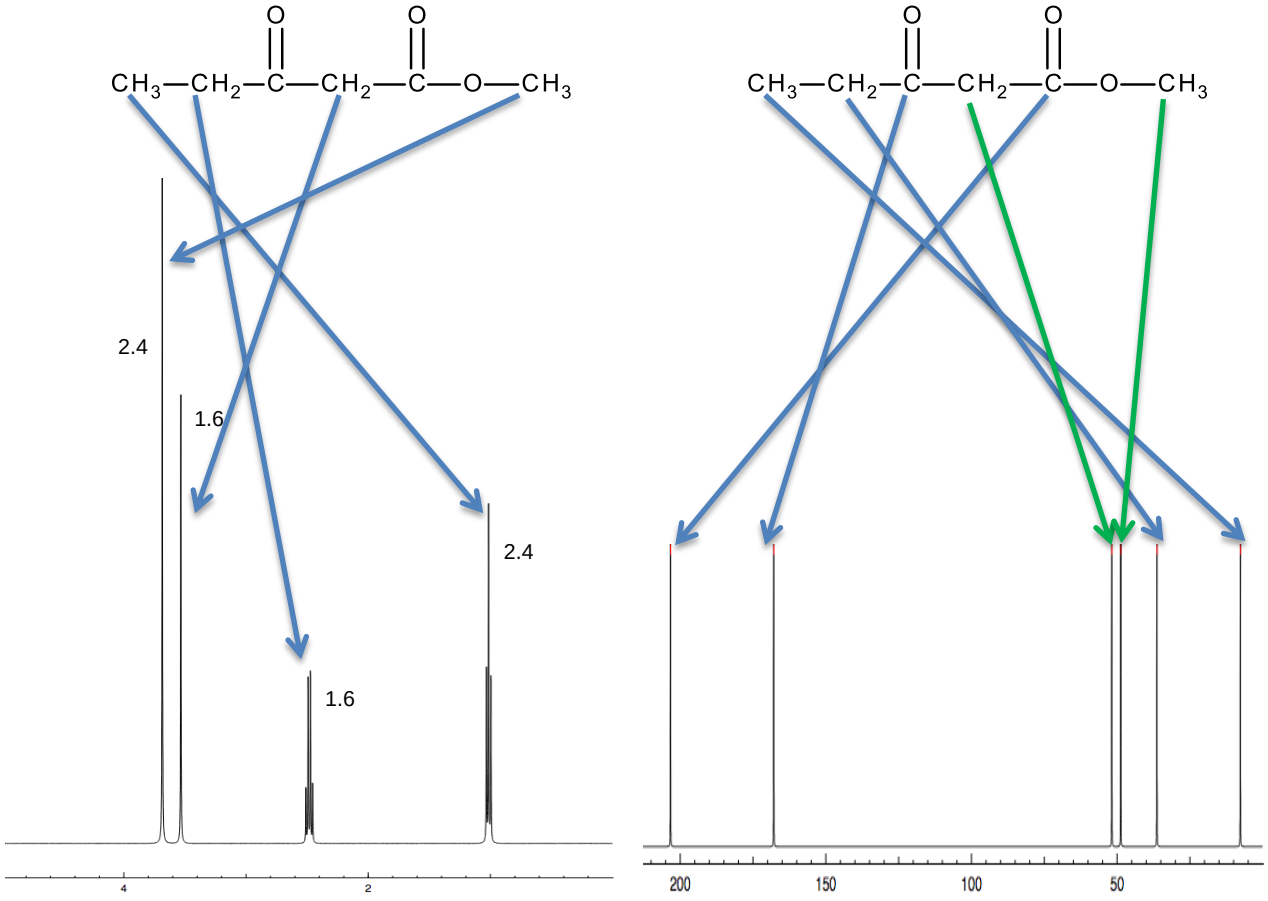


3 The ^{1}H and ^{13}C NMR spectra of $C_4H_8OBr_2$ are shown. Deduce the structure of the compound and then explain each signal.





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 →