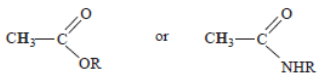
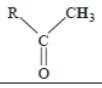
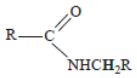
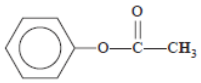
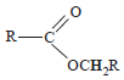
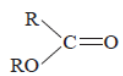
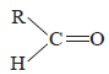
Ongoing revision – organic pathways, percentage yield, percentage atom economy and NMR

Type of proton	Chemical shift (ppm)
R–CH_3	0.9–1.0
R–CH_2–R	1.3–1.4
RCH=CH–CH_3	1.6–1.9
R_3–CH	1.5
	2.0
	2.1–2.7
R–CH_2–X (X = F, Cl, Br or I)	3.0–4.5
R–CH_2–OH, R_2–CH–OH	3.3–4.5
	3.2
R—O—CH_3 or R—O—CH_2R	3.3–3.7
	2.3
	3.7–4.8

Type of carbon	Chemical shift (ppm)
R–CH_3	8–25
R–CH_2–R	20–45
R_3–CH	40–60
R_4–C	36–45
R–CH_2–X	15–80
R_3C–NH_2, R_3C–NR	35–70
R–CH_2–OH	50–90
RC≡CR	75–95
R_2C=CR_2	110–150
RCOOH	160–185
	165–175
	190–200
R_2C=O	205–220

1) A compound has the molecular formula $C_5H_{10}O_2$. It's ^{1}HNMR spectrum contains the following splitting patterns and the chemical shift of each signal in ppm.

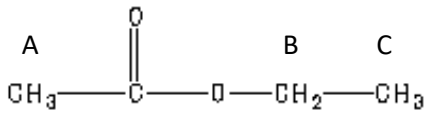
ppm	2.18	2.59	3.33	3.64
Splitting pattern	singlet	triplet	singlet	triplet
Integration value	3	2	3	2

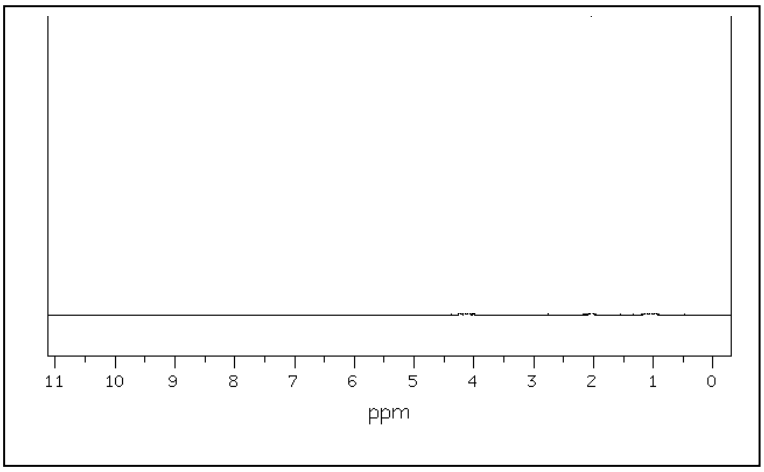
a) With reference to information on page 1 discuss what type of protons could have produced the singlets at 3.33 ppm and at 2.18 ppm

b) With reference to information on page 1 discuss what type of protons could have produced the triplets at 2.59 ppm and at 3.64 ppm

c) Draw the structural formula of the compound.

2) Consider the compound shown on the right.
a) With the information on page 1 draw a ^{1}HNMR spectrum for this compound showing the splitting pattern of each signal and its chemical shift in ppm.





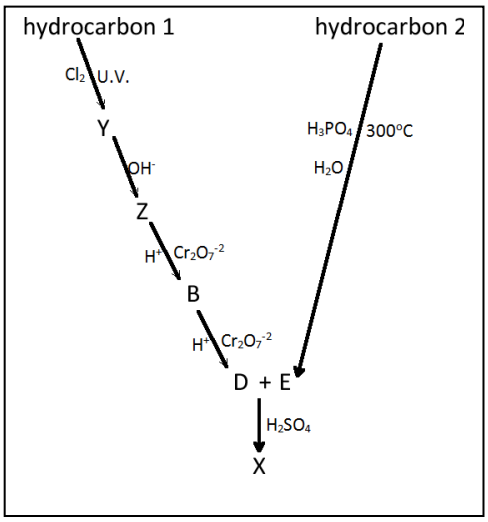
b) How many signals would appear on the ^{13}CNMR spectrum?

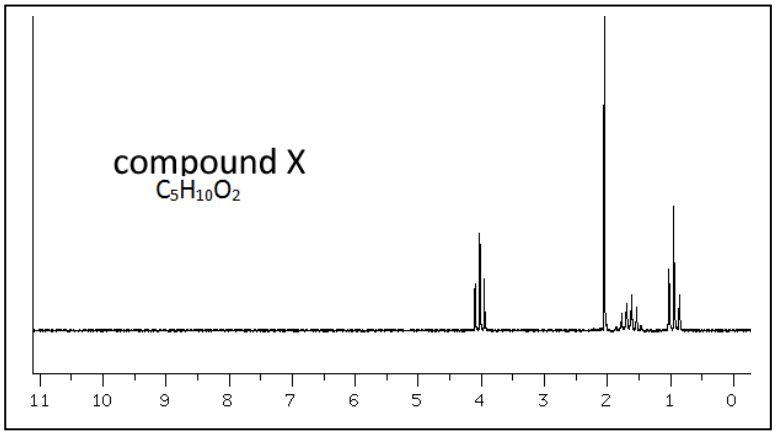
c) Would a signal appear at 205 ppm or at 170 ppm? Explain.

3) Consider the reaction pathways shown on the right to form compound X.

The ^{1}HNMR of compound X is shown below.

a) Identify compound X and draw its structural formula.





b) Identify the following.

Hydrocarbon 1 =

Hydrocarbon 2 =

Y =

Z =

B =

D =

E =

c) Compound E has other isomers. Name the other isomer.

d) What is the percentage atom economy of the reaction below?

hydrocarbon 2 → E

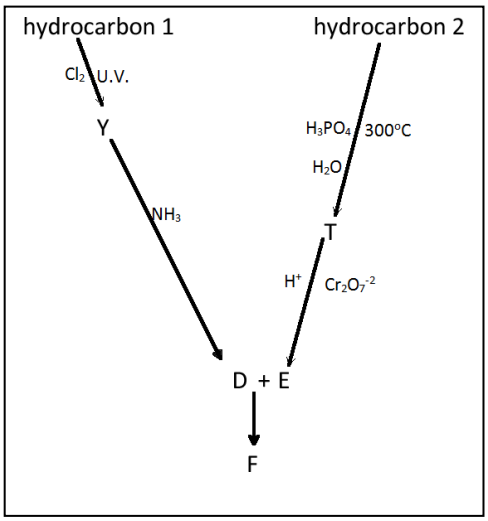
e) 12.2 grams of compound E was mixed with compound D to produce 16.1 grams of compound X. What is the percentage yield of the reaction below?

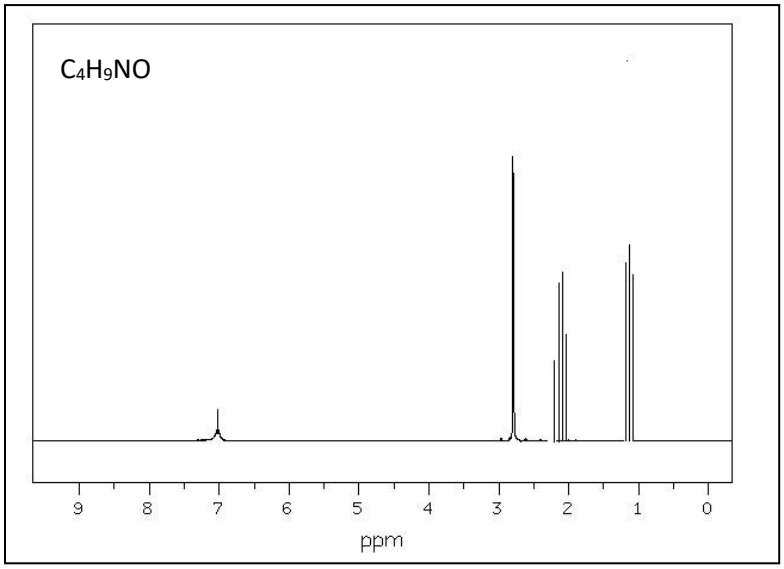
E + D → X

4) Consider the reaction pathways shown on the right to form compound F.

The ^{1}HNMR spectrum of compound F is shown below

a) Draw the structural formula of "F".





b) Identify the following.

Hydrocarbon 1 =

Hydrocarbon 2 =

Y =

D =

E =

T =

c) What type of reaction is D + E → F?