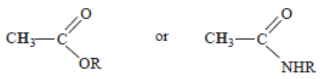
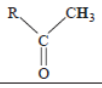
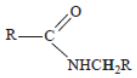
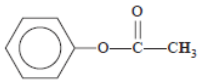
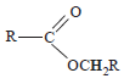
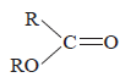
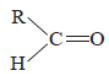
Ongoing revision – organic pathways, percentage yield, percentage atom economy and NMR

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

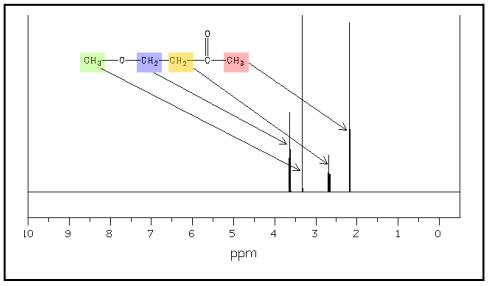
a) With reference to information on page 1 discuss what type of protons could have produced the singlets at 3.33 ppm and at 2.18 ppm

Two CH_3 groups without neighbouring hydrogens

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

Two CH_2 groups next to each other without neighbouring hydrogens

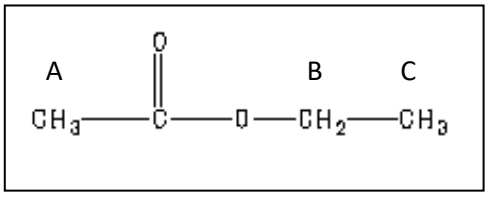
$-CH_2 - CH_2 -$

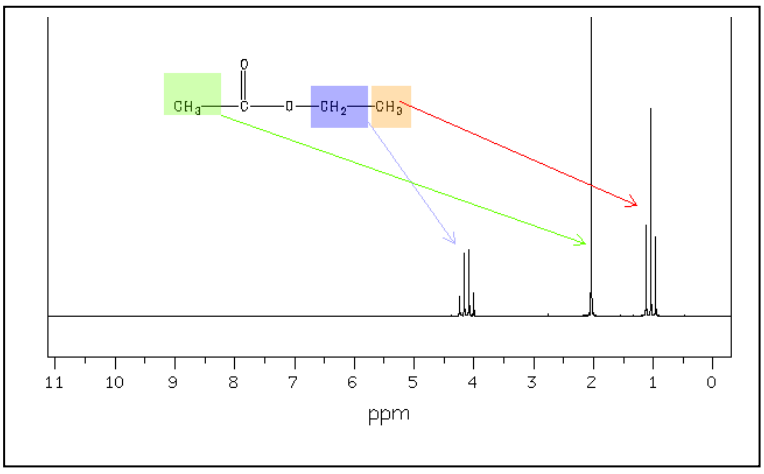


c) Draw the structural formula of the compound.

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?

4

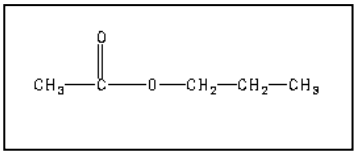
c) Would a signal appear at 205 ppm or at 170 ppm? Explain.

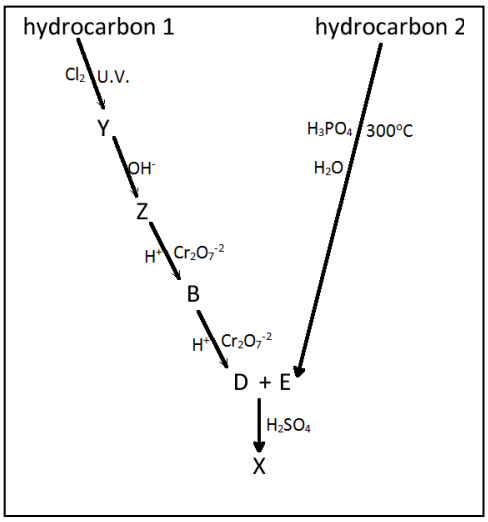
A signal at 205 ppm indicates a ketone($R_2C=O$) group, according to the data sheet. A peak at 170 indicates an ester functional group $RCOOR_1$.

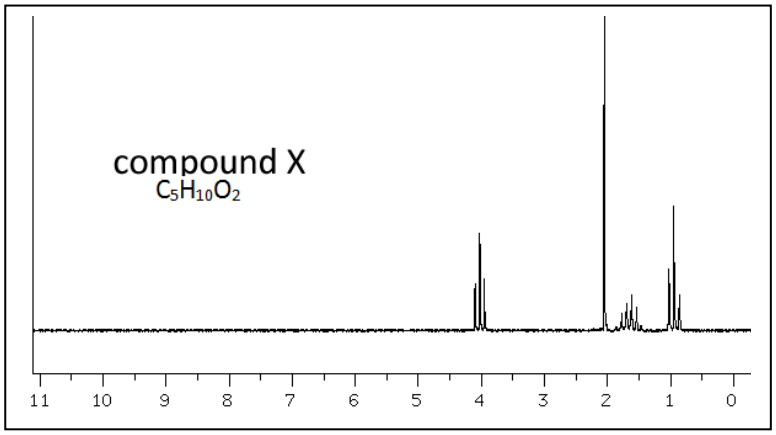
3) Consider the reaction pathways shown on the right to form compound X.

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

a) Identify compound X and draw its structural formula. *Propyl ethanoate*







b) Identify the following.

Hydrocarbon 1 = *ethane*

Hydrocarbon 2 = *prop-1-ene*

Y = *chloroethane*

Z = *ethanol*

B = *ethanal (naming of aldehydes is not required in this course)*

D = *ethanoic acid.*

E = *propan-1-ol*

c) Compound E has other isomers. Name the other isomer. *Propan-2-ol*

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

hydrocarbon 2 → 100%

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

Step 1 find the mol of E.

=> E is propanol with a molar mass of 60.1 => 12.2 / 60.1 = 0.203 mol

Step 2 find the theoretical amount of X formed

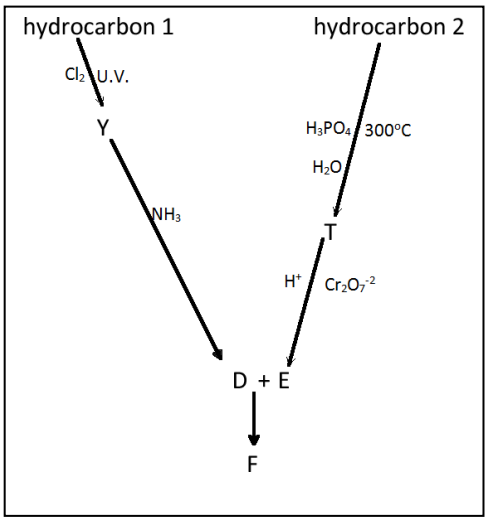
=> 0.203 X molar mass of propyl ethanoate

=> 102.1 X 0.203 = 20.7 grams

Step 3 find the percentage yield

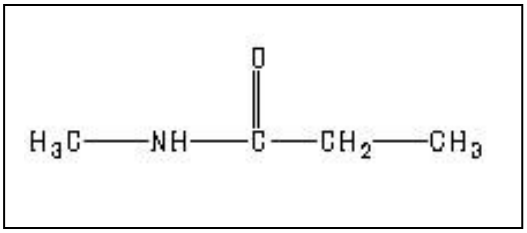
=> (16.1 / 20.7) X 100 = 77.8%

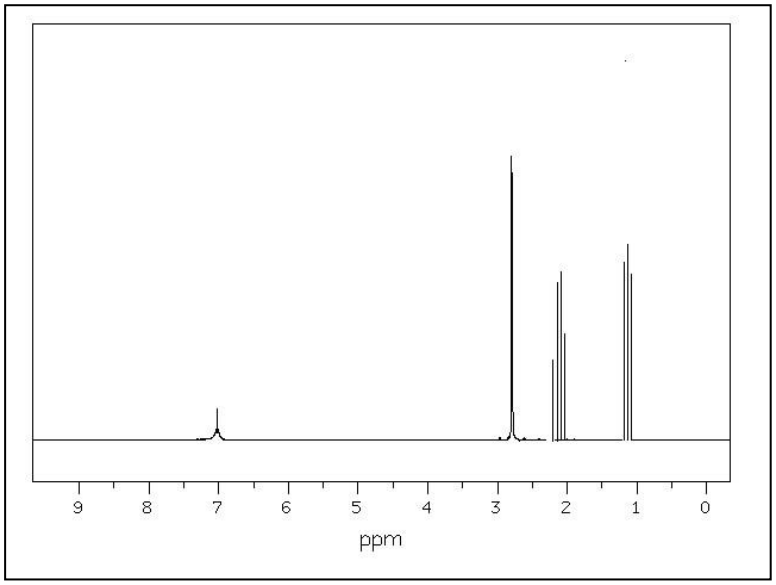
4) Consider the reaction pathways shown on the right to form compound F.



5)

a) Draw the structural formula of "F".





b) Identify the following.

Hydrocarbon 1 = *methane*

Hydrocarbon 2 = *propene*

Y = *chloromethane*

D = *methanamine*

E = *propanoic acid*

T = *propan-1-ol*

c) What type of reaction is D + E → F? *Condensation reaction or esterification*