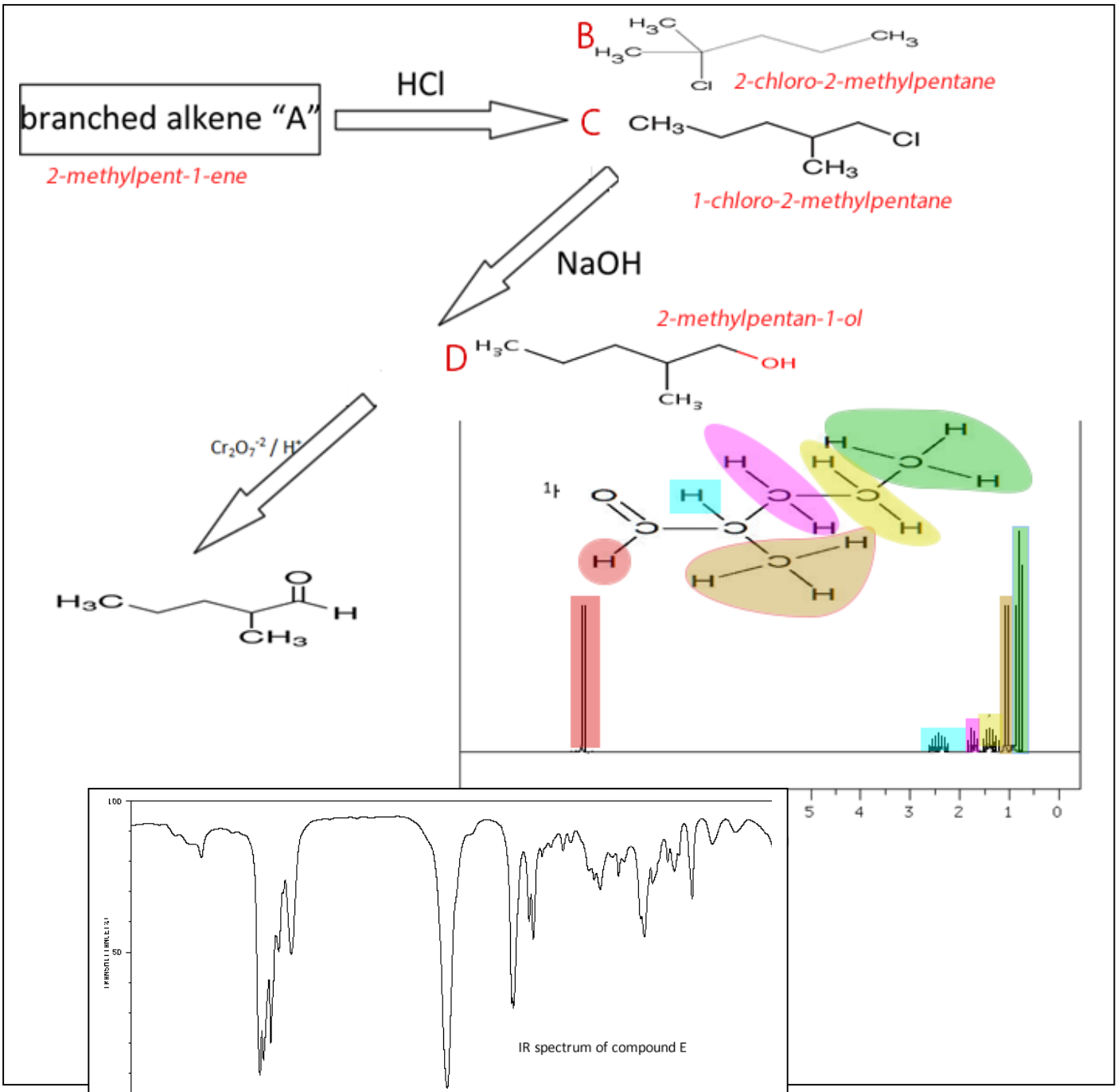
Friday worksheet – organic pathways, naming organic compounds and spectroscopy

1) A branched alkene with molecular formula C_6H_{12} is used to produce compound E via the reaction pathway shown below.
   a) Draw the structural formula of compound E given the information below.
   b) Name and draw the structural formulae of the compounds D, C and B in the spaces below.
   c) Give the systematic name of compound A.



d) After looking at the IR spectrum above of compound E a student suggested it could be either an acid, a ketone or an aldehyde.

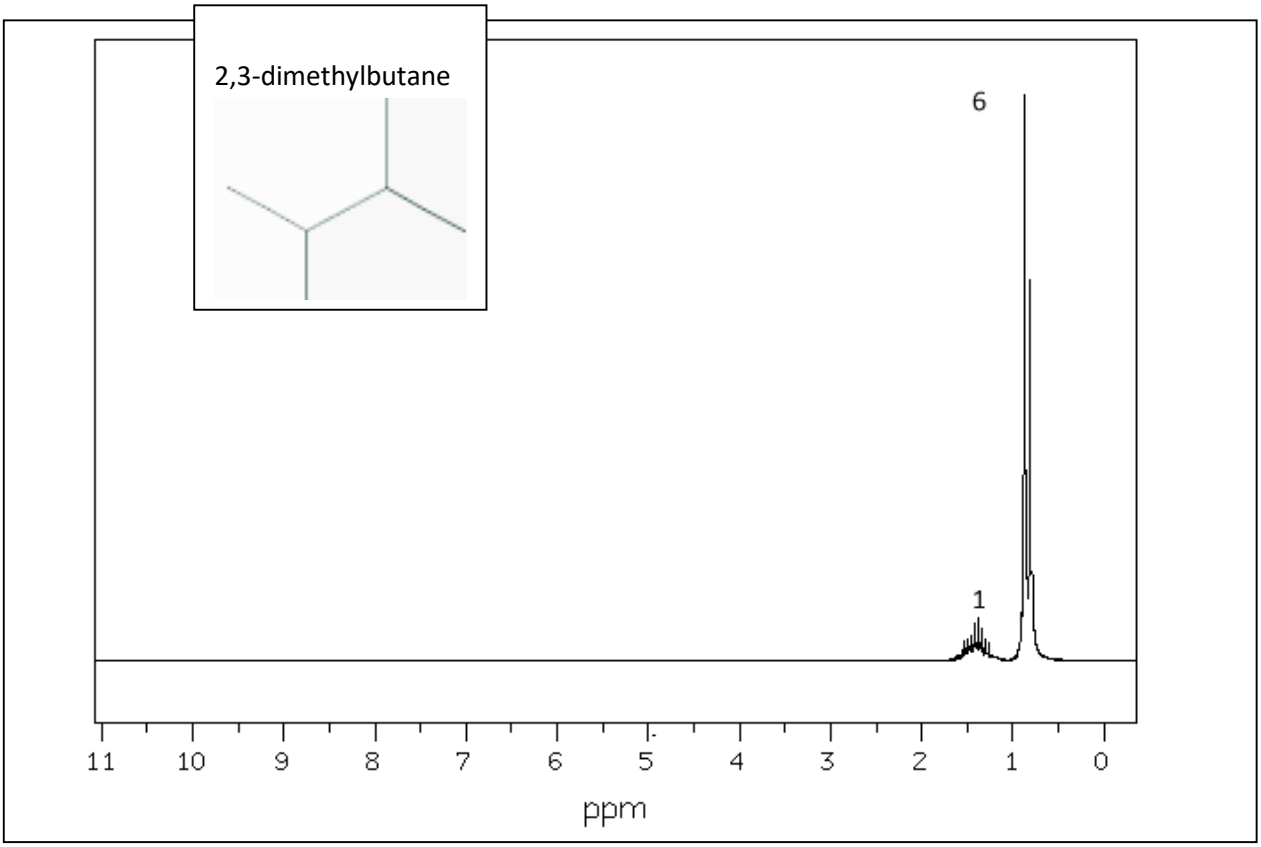
i. Suggest a reason why the student came to that conclusion.

A high absorbance around 1700 cm^{-} indicates an C=O bond of either an aldehyde, carboxylic acid or ketone.

ii. Suggest to which group of organic compounds, mentioned by the student in question i. above, does compound E NOT belong to. Give a reason for your answer.

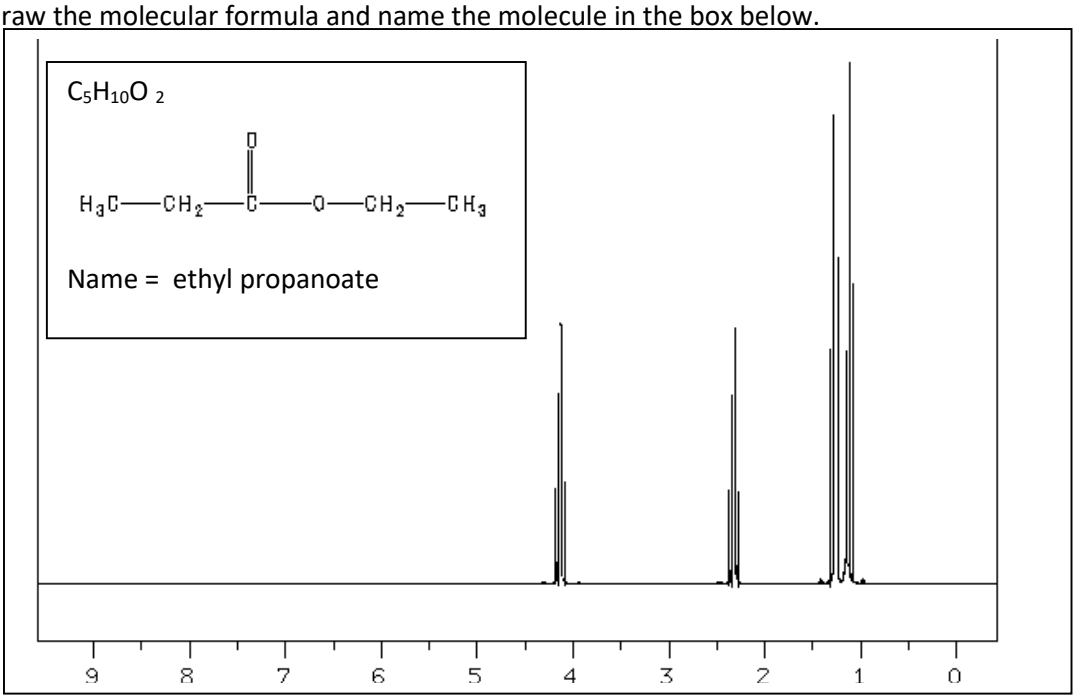
Compound E is not a carboxylic acid. There is an absence of a broad trough between 2500-3500 characteristic of an acidic O-H absorbance.

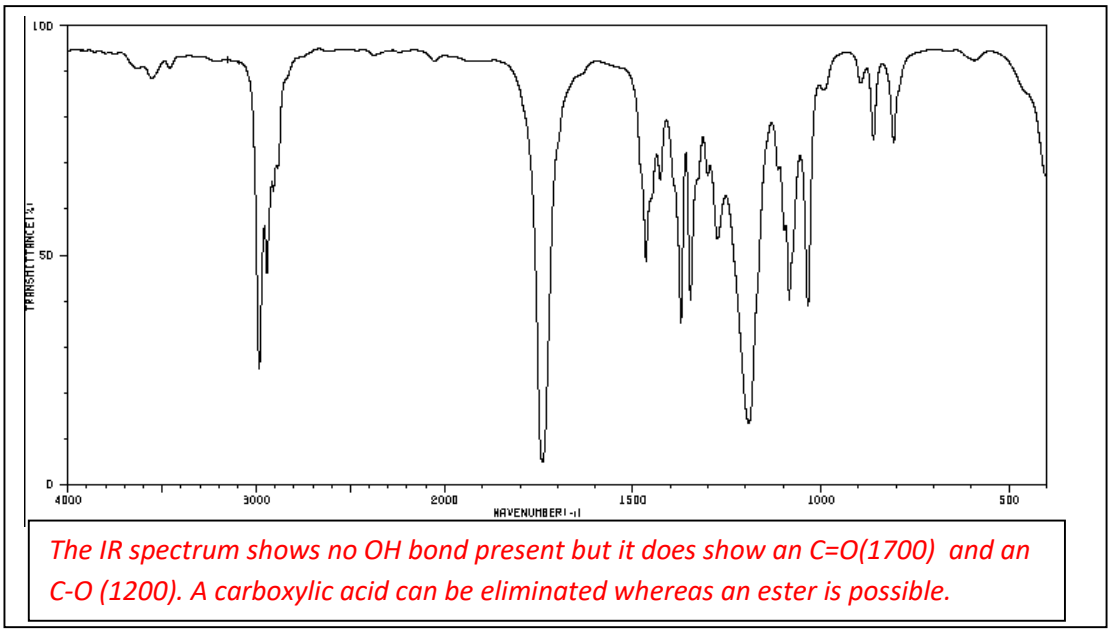
2) A compound with the formula C_6H_{14} has the ^{1}HNMR spectrum shown below. Identify the compound using the n+1 rule and draw its skeletal structure in the space provided.
Note – this spectrum has been slightly modified for the n+1 rule. The signal at 1.4 ppm is split into more peaks than are shown on the spectrum. The simplest ratio of the area under each peak is also shown.



3) The ^{1}HNMR and the IR spectra of a compound with the molecular formula $C_5H_{10}O_2$ are shown below.

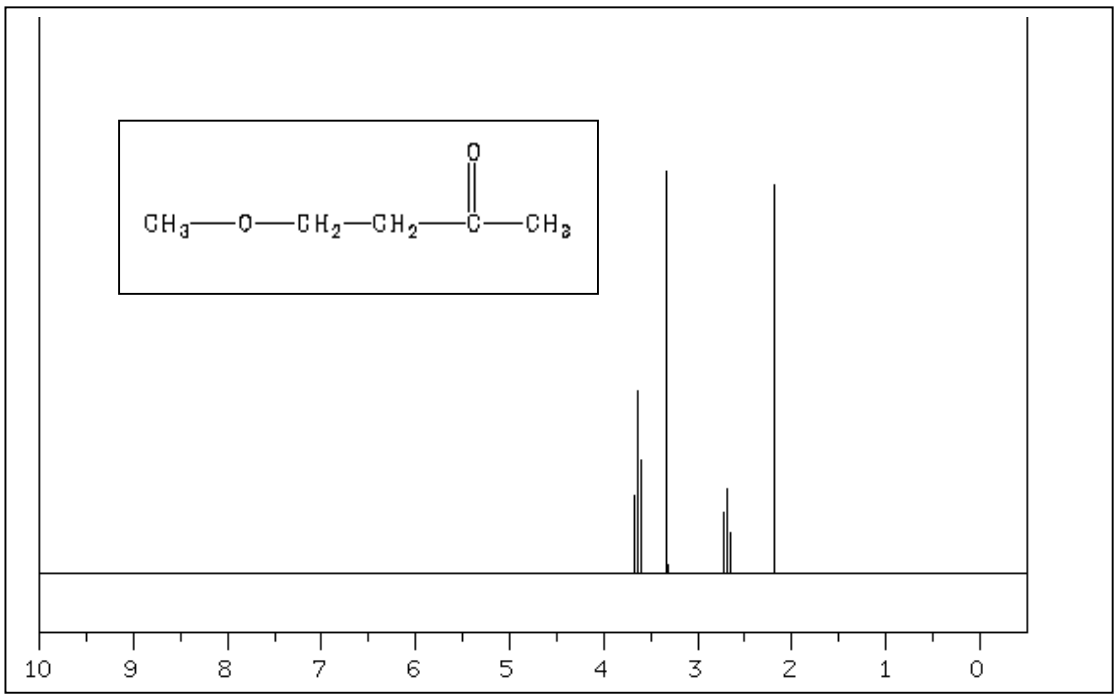
a) Draw the molecular formula and name the molecule in the box below.

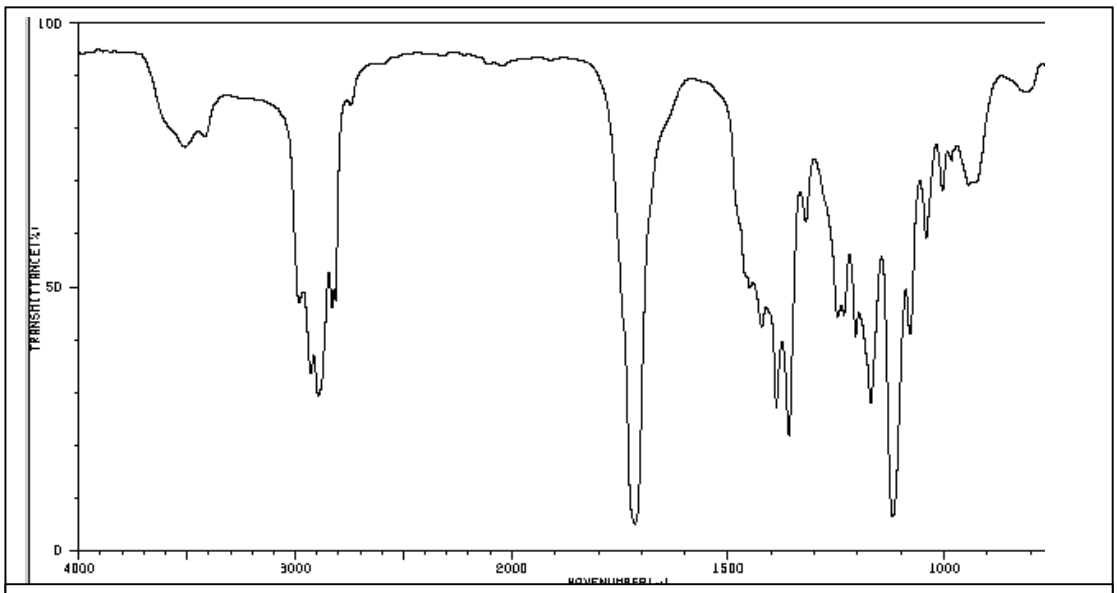




The IR spectrum shows no OH bond present but it does show an C=O(1700) and an C-O (1200). A carboxylic acid can be eliminated whereas an ester is possible.

b) Consider a compound with the same molecular formula ($C_5H_{10}O_2$) as the compound in a) above. It's IR and ^{1}HNMR spectra are shown below. Draw it's molecular formula.





The IR spectrum shows no indication of an OH bond so acid and alcohol can be ruled out. There is an indication that a C=O and C-O are present. Knowing this we could be looking to form a molecule with a combination of a ketone or aldehyde group as well as an ether functional group. The ^{1}HNMR spectrum shows four chemically different hydrogen environments and two large singlets, that <u>maybe</u> due to two isolated CH_3 groups present. The two triplets may be due to two CH_2 groups next to each other. Use the data booklet for the NMR ppm numbers to verify type of protons environments.

*- an R-CO-**CH_3** appears at 2.1 and 2.7 ppm. This is confirmed by the spectrum.*

*- an R-O-**CH_2**-R appears at 3.3 -3.7 ppm This is confirmed by the spectrum.*

*- an R-O-**CH_3** also appears at 3.3 -3.7 ppm. This is also confirmed by the spectrum*