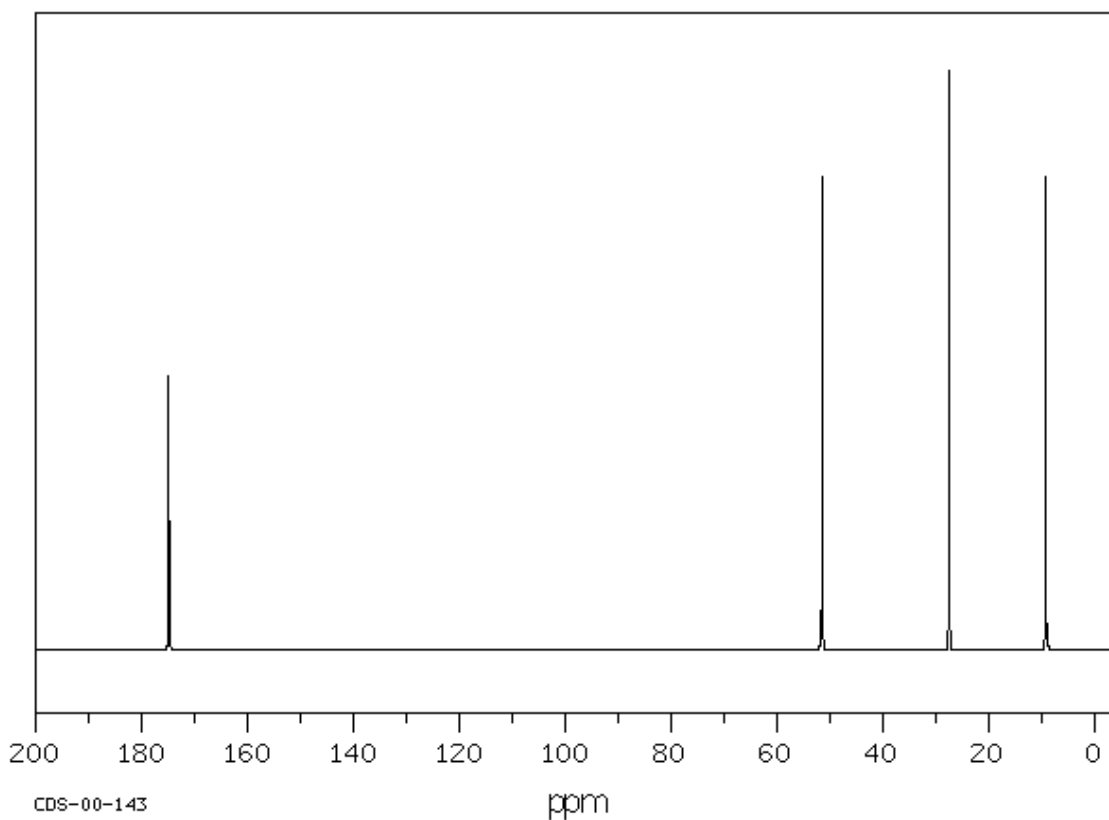


Chemguide – questions

C-13 NMR: INTERPRETING SPECTRA

1. The two isomers of C_2H_6O are ethanol, CH_3CH_2OH , and methoxymethane, CH_3OCH_3 . Describe as fully as you can what the C-13 NMR spectra of the two compounds would look like. You will find a table of chemical shift values on the final page of these questions.
2. The C-13 NMR spectrum for methyl propanoate, $CH_3CH_2COOCH_3$, is given below. All the spectra in this file are taken from the SDBS (SDBSWeb : <http://sdb.sdb.aist.go.jp> (National Institute of Advanced Industrial Science and Technology, 20/8/2014)).

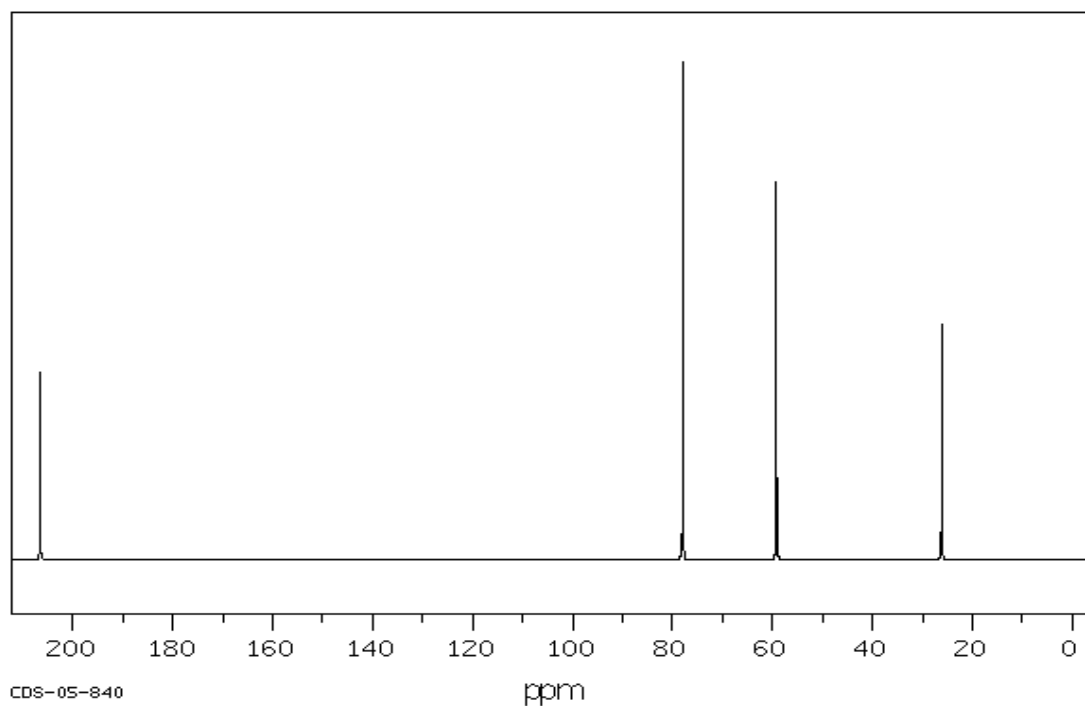


Decide which carbon atoms in the methyl propanoate are responsible for each of the lines in the spectrum.

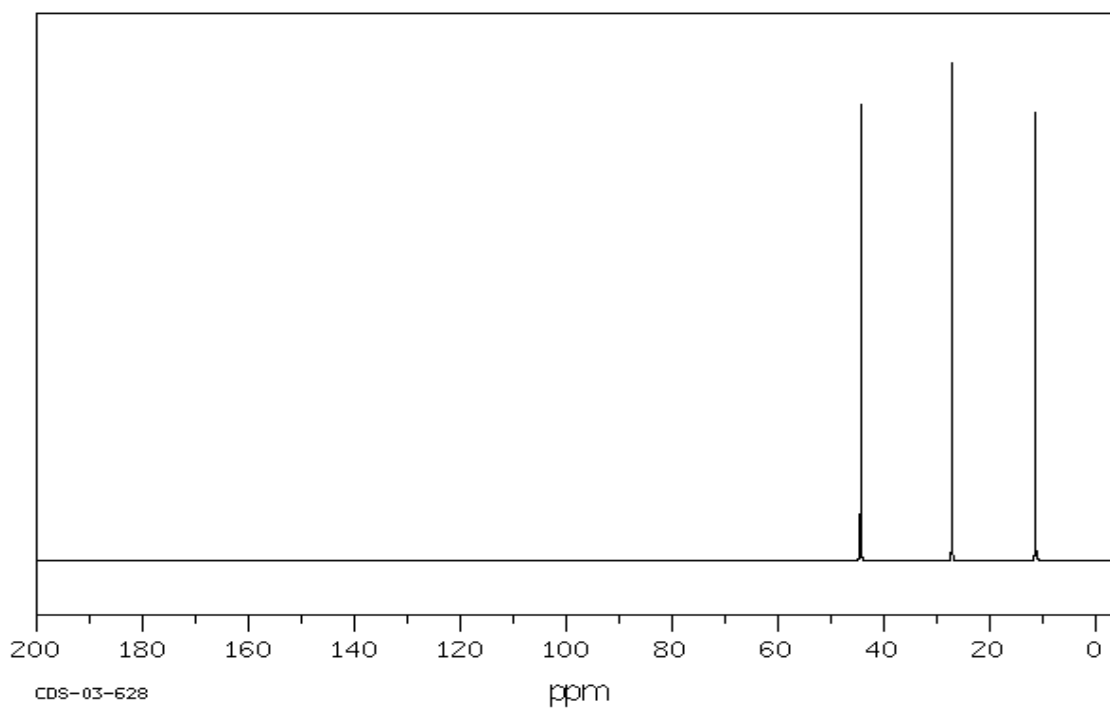
questions continue . . .

Chemguide – questions

3. An isomer of methyl propanoate has the following C-13 NMR spectrum. Work out the probable structural formula for the compound, explaining your reasoning.



4. A compound with a relative molecular mass of 59 gave the following C-13 NMR spectrum. Suggest the identity of the compound.



(Note: One of the chemical shifts is *slightly* different from the value given in the table.)

Chemguide – questions

carbon environment	chemical shift (ppm)
C=O (in ketones)	205 - 220
C=O (in aldehydes)	190 - 200
C=O (in acids and esters)	160 - 185
C in aromatic rings	125 - 150
C=C (in alkenes)	115 - 140
RCH ₂ O-	50 - 90
RCH ₂ Cl	30 - 60
RCH ₂ NH ₂	30 - 65
R ₃ CH	25 - 35
CH ₃ CO-	20 - 50
R ₂ CH ₂	16 - 25
RCH ₃	10 - 15