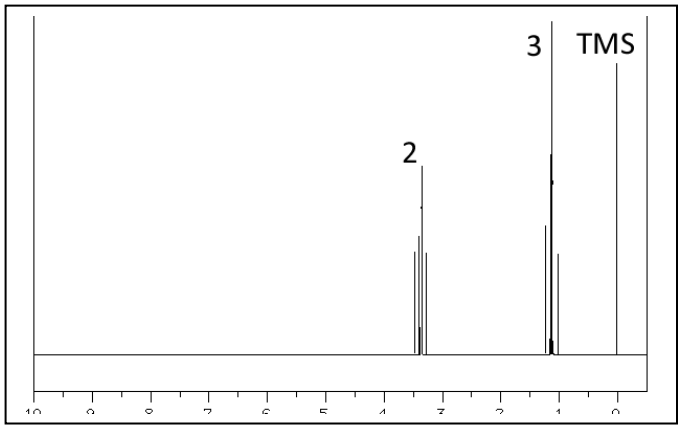
Lesson 3 ^{1}HNMR

1) A compound has the molecular formula $C_4H_{10}O$
Its ^{1}HNMR spectrum is shown on the right.
Students were given this information and asked to identify the compound.



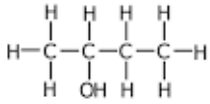
a) How many non-equivalent hydrogens exist. *2*

b) A student offered the following possible compounds.

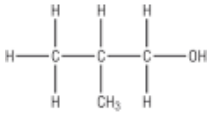
i. butan-2-ol
ii. 2-methylpropan-1-ol
iii. 1-butanol
iv. 2-methylpropan-2-ol

Draw the structural formulae of the compounds and give a reason why each compound is or is not represented by the spectrum above.

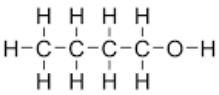
butan-2-ol



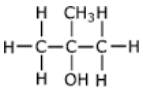
2-methylpropan-1-ol



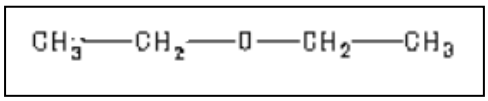
butan-1-ol



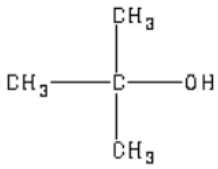
2-methylpropan-2-ol



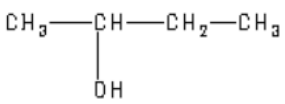
c) Draw the structural formula of the compound represented by the ^{1}HNMR spectrum above.



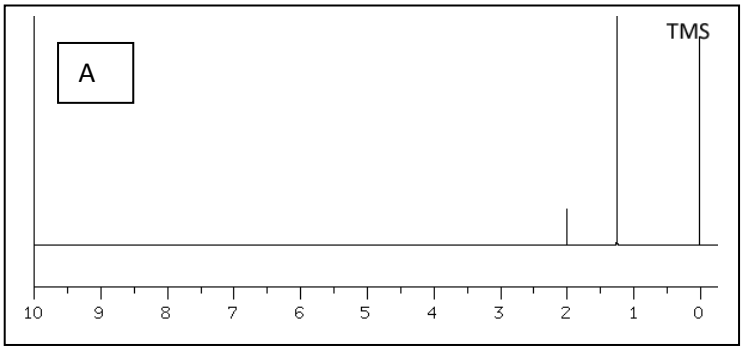
2) The two spectra below, belong to two of the compounds listed above. Identify the compounds

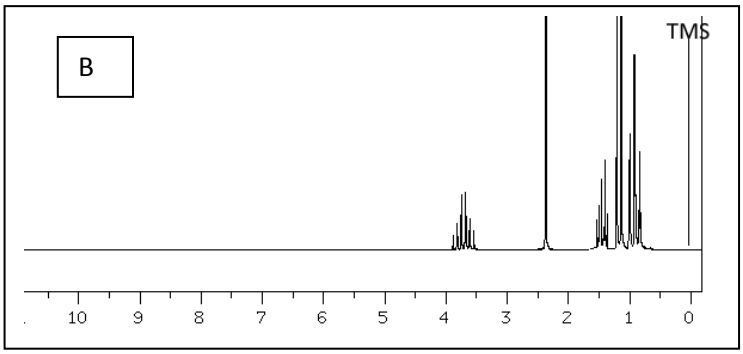


2-methyl-2-propanol = A



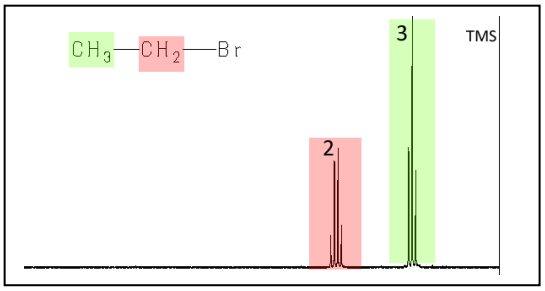
butan-2-ol = B





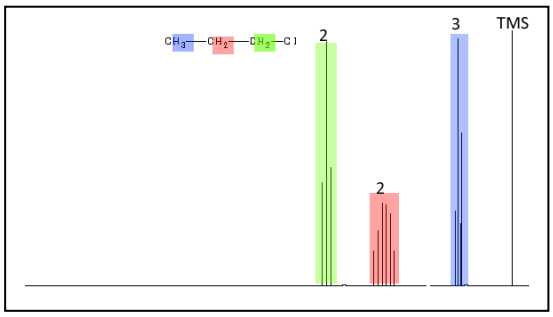
3) On the set of axes below draw the possible splitting patterns in their relative order to form a ^{1}HNMR spectrum. Predict the area under each peak for each spectrum.

a) 1-bromoethane



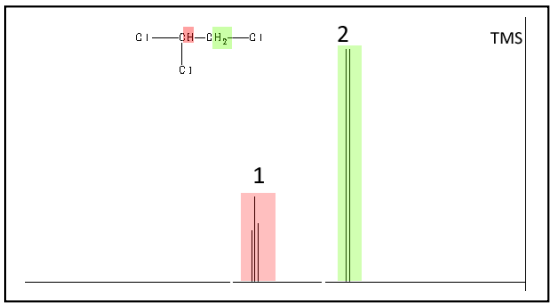
There should be only two peaks since there are only two non-equivalent hydrogens. The splitting pattern should have a triplet and a quartet. The CH_2 next to the Br is less shielded so it should appear with a greater chemical shift than the terminal CH_3.

b) 1-chloropropane



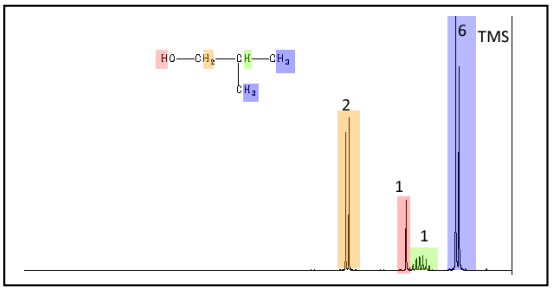
There should be only three peaks since there are only 3 non-equivalent hydrogens. The splitting pattern should have two triplets and a sextet. The CH_2 next to the Cl is less shielded so it should appear with a greater chemical shift than the terminal CH_3.

c) 1,1,2-trichloroethane



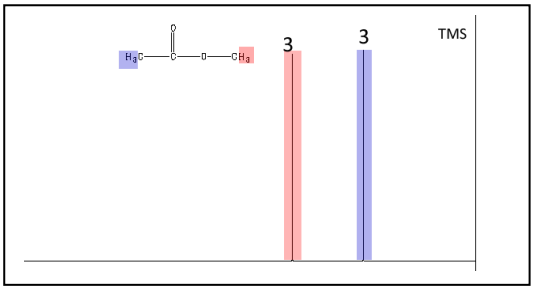
There should be only two peaks since there are only 2 non-equivalent hydrogens. The splitting pattern should have a triplet and a doublet. The CH next to the 2 Cl atoms is less shielded so it should appear with a greater chemical shift than the terminal CH_2(in green)

d) 2-methyl-1-propanol



There should be only four peaks since there are only 4 non-equivalent hydrogens.
The splitting pattern should have two doublets, a singlet and a nonet.
The order in which the peaks appear was not obvious and students were not expected to get the exact order correct.

e) methyl ethanoate



There should be only two peaks since there are only 2 non-equivalent hydrogens.
The splitting pattern should have two singlets.
The CH_3 next to the oxygen atom is less shielded so it should appear with a greater chemical shift than the terminal CH_3(in blue)