

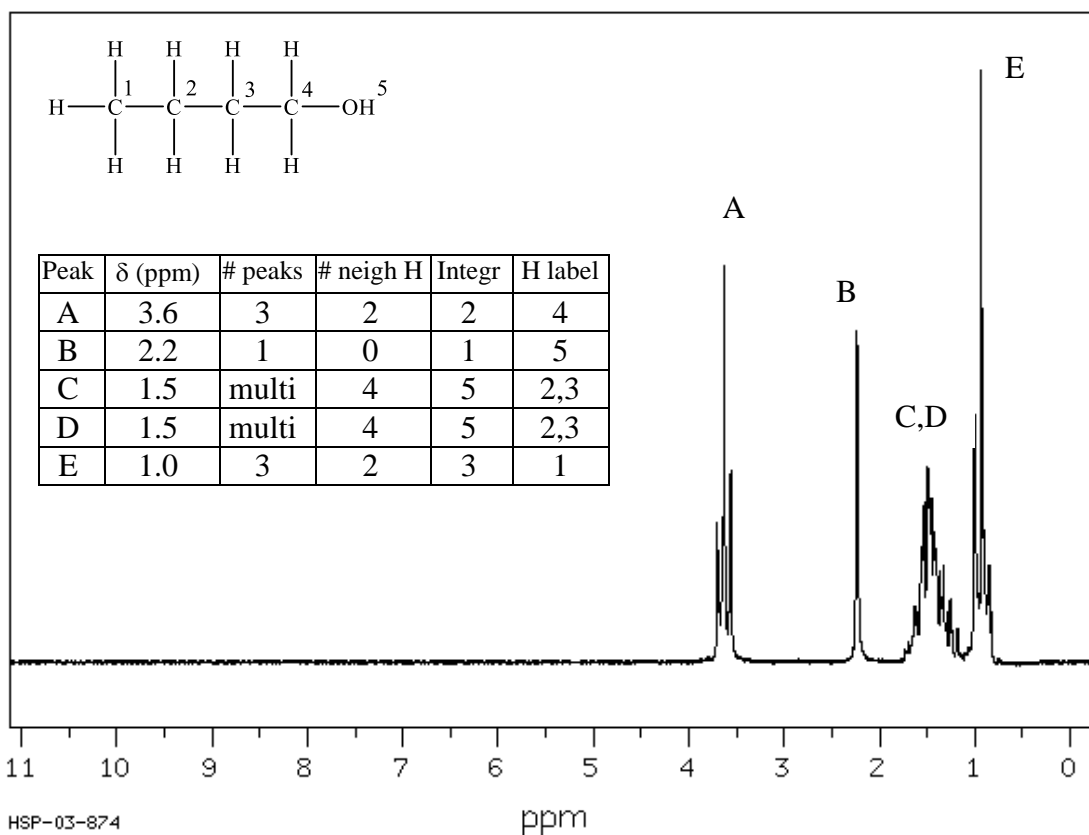
### Homework 3

1. The following proton spectra were obtained for compounds with the molecular formula of  $C_4H_{10}O$ . (Hint: There are just 7 structural isomers possible for this molecular formula - the  $(CH_3)_2CHOCH_3$  isomer's NMR is NOT shown.). We have not yet covered these structures yet, which include alcohols and ethers. You can think of an alcohol as an alkane with an oxygen atom inserted between a carbon atom and a hydrogen atom. An ether would have an oxygen atom inserted between two carbon atoms. Thus, for the alkane ethane,  $CH_3CH_3$ , the alcohol would be  $CH_3CH_2OH$  and the ether  $CH_3OCH_3$ .

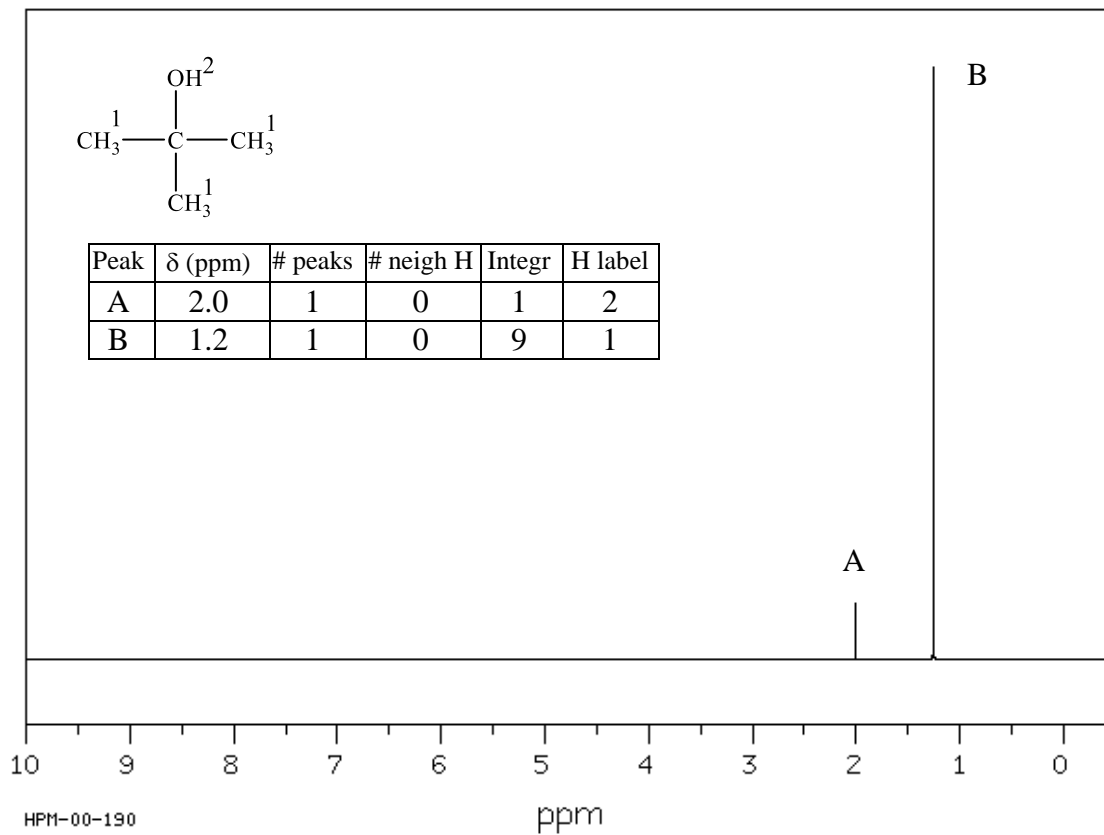
What is the structure of each compound? Make a summary table for each and list the approximate chemical shift, the number of peaks, number of neighboring protons, and the integration of the peak.

\*Remember that in decoupled  $^{13}C$  NMR, a "peak" is just a single line (or absorption) but in  $^1H$  NMR a "peak" is usually a group of peaks (multiplet), but can be a singlet. Thus, in  $^1H$  NMR spectroscopy, overlapping "peaks" usually visually complicated.

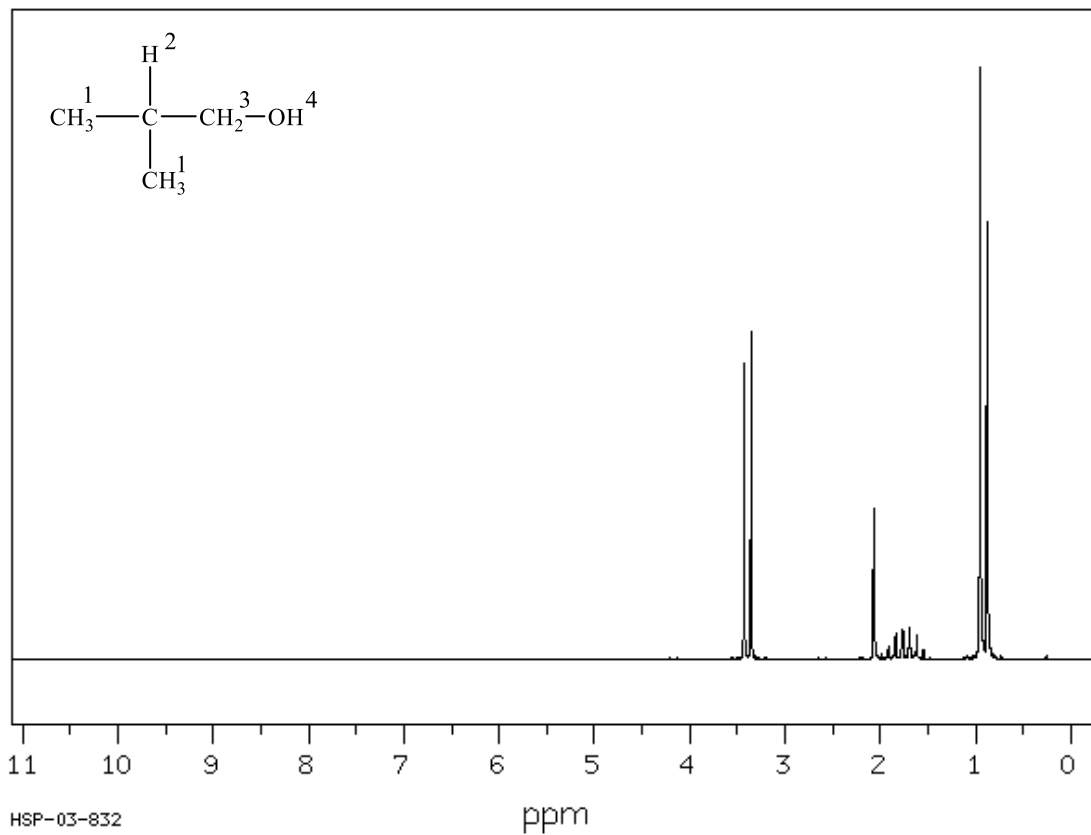
Spectrum A: Two peaks overlap at 1.4 ppm



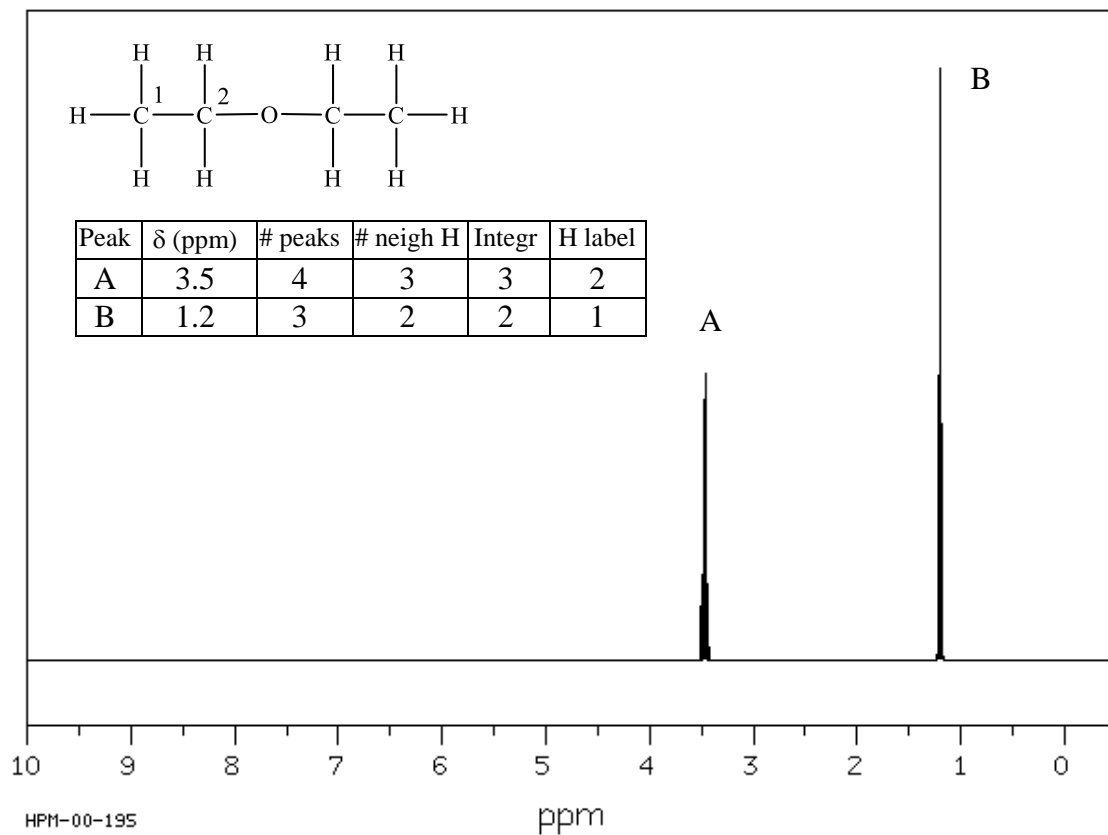
Spectrum B:



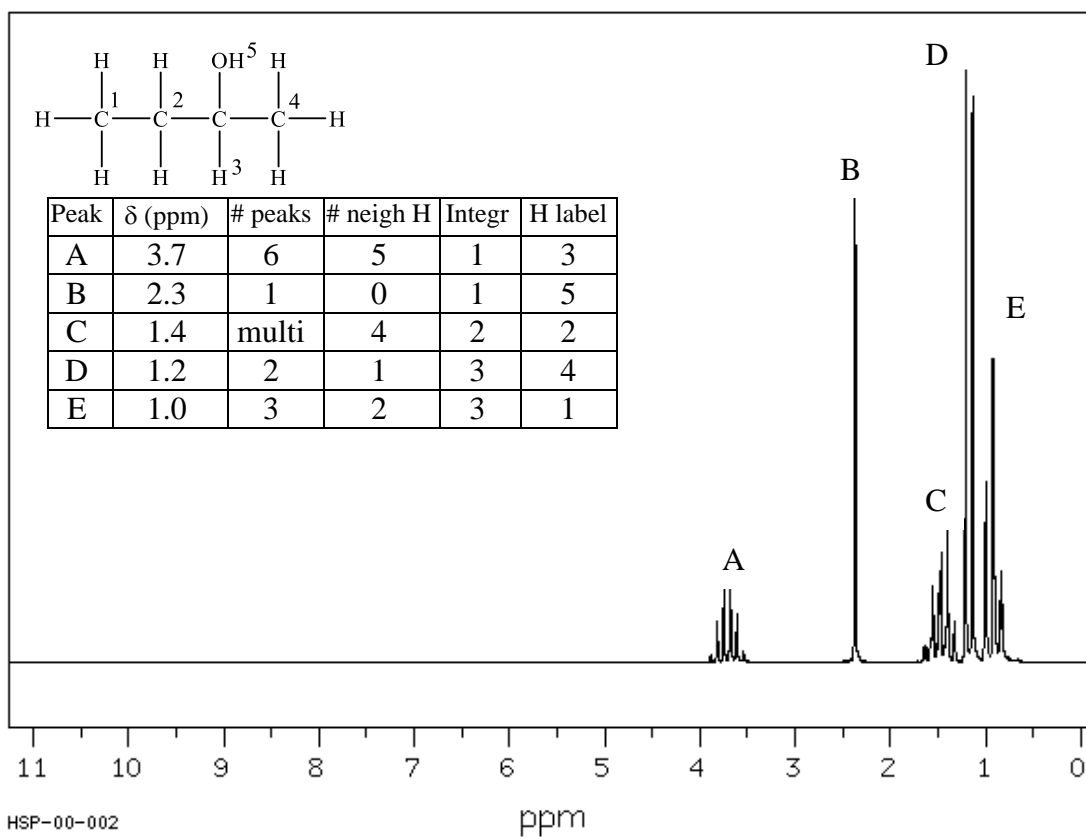
Spectrum C:



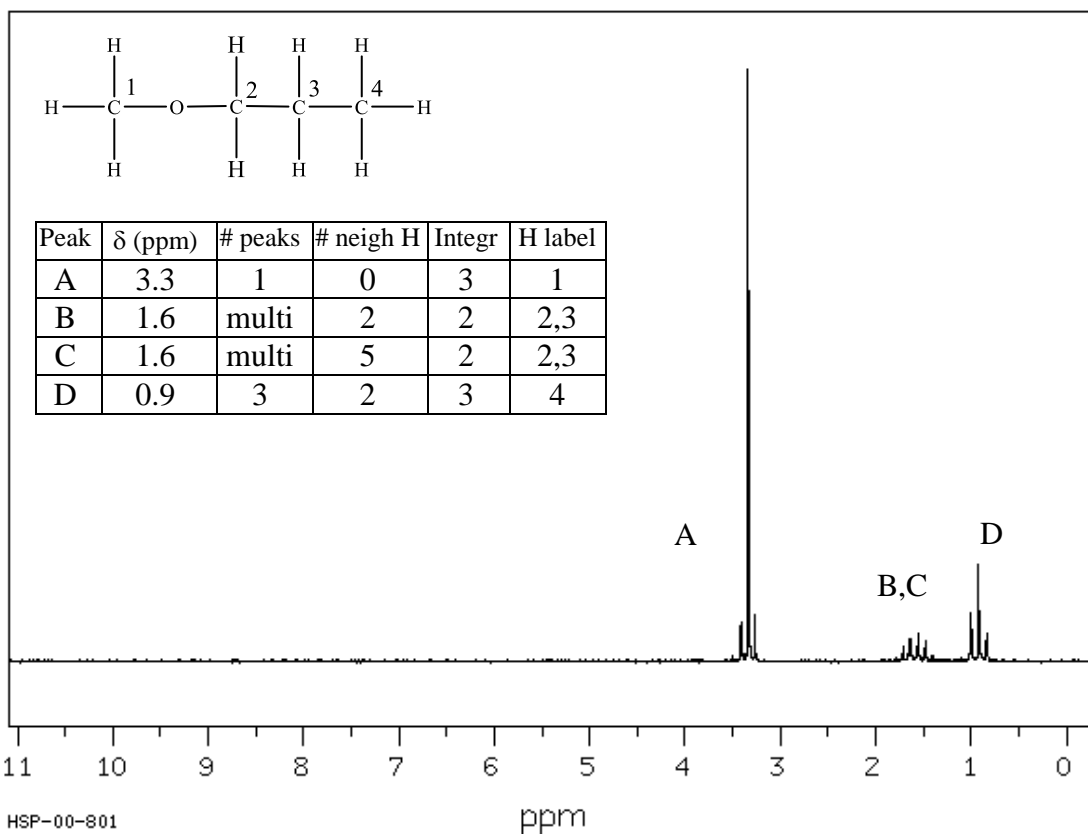
Spectrum D:



Spectrum E:



Spectrum F: Two peaks are overlapping at 3.34 ppm



2. Solve the following structures from their proton spectra:

Molecular Formula	chemical shifts (multiplicity, integration) multiplicity: d-doublet, t-triplet, q-quartet, m-multiplet
a) $C_7H_8O$	2.43 (s, 1), 4.58 (s, 2), 7.28 (m, 5)
b) $C_4H_8Br_2$	1.9 (s, 6), 3.9 (s, 2)
c) $C_3H_7Br$	1.1 (t, 3), 1.9 (m, 2), 3.4 (t, 2)
d) $C_{11}H_{16}$	1.2 (s, 9), 2.3 (s, 3), 7.2 (m, 4)
e) $C_4H_{10}O$	1.2 (t, 3), 3.5 (q, 2)
f) $C_4H_8O_2$	1.3 (t, 3), 2.0 (s, 3), 4.1 (q, 2)
g) $C_4H_8O_2$	1.0 (t, 3), 1.7 (m, 2), 2.3 (t, 2), 11.5 (s, 1)

- a) benzyl alcohol
- b) 1,2-dibromo-2-methylpropane
- c) 1-bromopropane
- d) tert-butyltoluene (could be ortho, meta, or para from the information given)
- e) diethylether
- f) ethyl acetate
- g) butanoic acid