

Chemguide – questions

H-1 NMR: LOW RESOLUTION

The spectral data in this file are taken from the SDBS (SDBSWeb : <http://sdb.db.aist.go.jp> (National Institute of Advanced Industrial Science and Technology, 26/8/2014).

1. For the tables of low resolution ^1H NMR data below, work out the structure of the molecules concerned. You will find a short table of useful chemical shifts at the bottom of the page.

I am giving you tables of data rather than spectra, because I can't find any reliable source of real low resolution NMR spectra.

a) A molecule with the molecular formula $\text{C}_3\text{H}_6\text{O}_2$ which gave this pattern of peaks:

chemical shift (ppm)	11.73	2.380	1.159
ratio of areas under the peaks	1	2	3

b) A molecule with the molecular formula $\text{C}_4\text{H}_8\text{O}$ which gave this pattern of peaks:

chemical shift (ppm)	9.764	2.37	1.64	0.97
ratio of areas under the peaks	1	2	2	3

c) A molecule with the molecular formula $\text{C}_5\text{H}_{10}\text{O}_2$ which gave this pattern of peaks:

chemical shift (ppm)	4.132	2.319	1.259	1.140
ratio of areas under the peaks	2	2	3	3

Chemical shifts

	chemical shift, δ
$\text{R}-\text{CH}_3$	0.7 - 1.6
$\text{R}-\text{CH}_2-\overset{\text{O}}{\parallel}{\text{C}}-$	2.0 - 2.9
$-\text{O}-\text{CH}_3$ or $-\text{O}-\text{CH}_2-\text{R}$	3.3 - 4.3
$\overset{\text{O}}{\parallel}{\text{H}-\text{C}}-$	9.0 - 10.0
$-\text{COOH}$	11.0 - 12.0

(I have used the table of shifts from the Chemguide page to save time in redrawing the structures. The $\text{R}-\text{CH}_2-\text{R}$ group has shifts in the same region as the $\text{R}-\text{CH}_3$ group.)