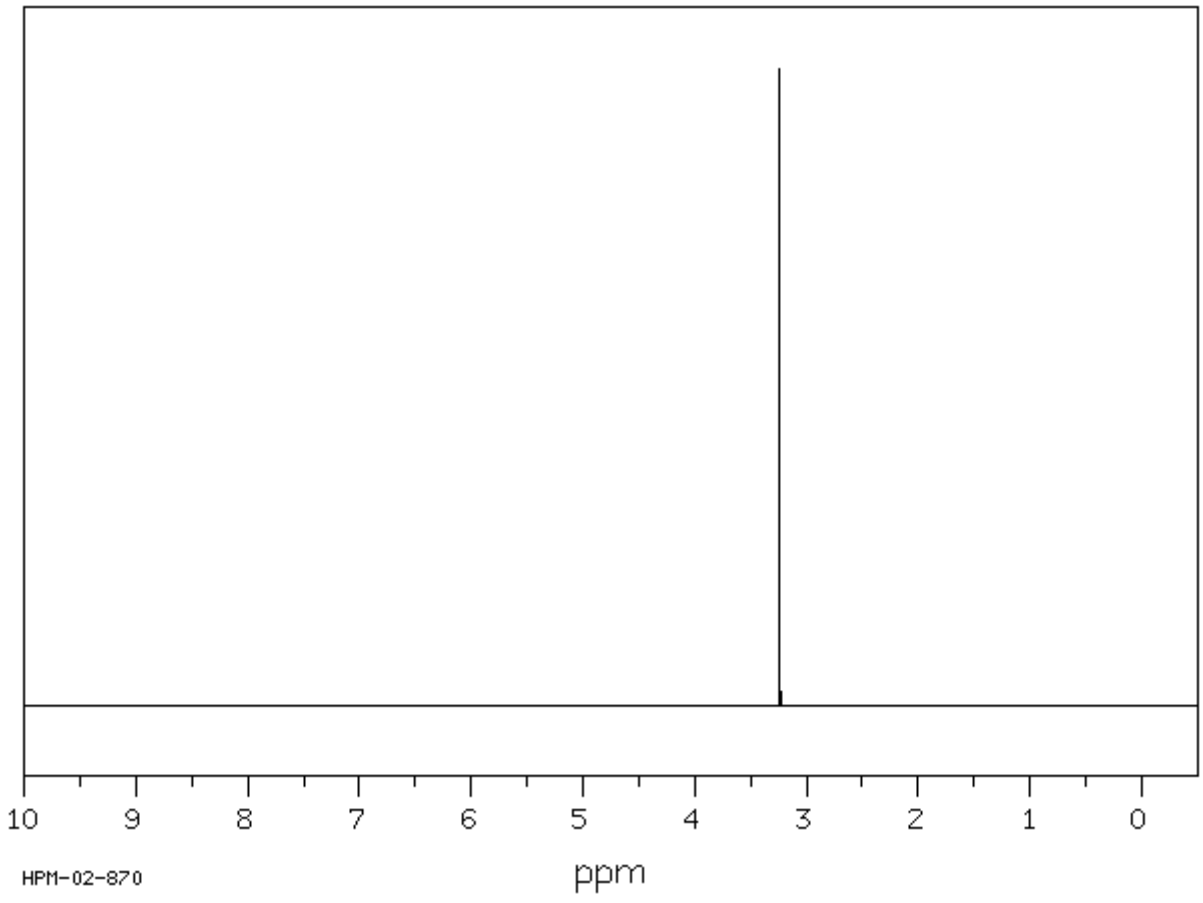
H-1 NMR: INTRODUCTION

1. ^1H atoms have a nucleus which can behave as a tiny magnet which will align with an external magnetic field. If you pass energy in the form of radio waves with a frequency of about 60 to 100 MHz through an organic compound containing hydrogen, for a particular magnetic field, the ^1H nuclei will flip constantly backwards and forwards from being aligned with the field to being aligned against it. This is known as the resonance condition for a particular hydrogen nucleus.

   a) For a given frequency of radio waves, why would the resonance condition for a hydrogen atom attached to a carbon atom need a slightly different external magnetic field from one attached to an oxygen atom?

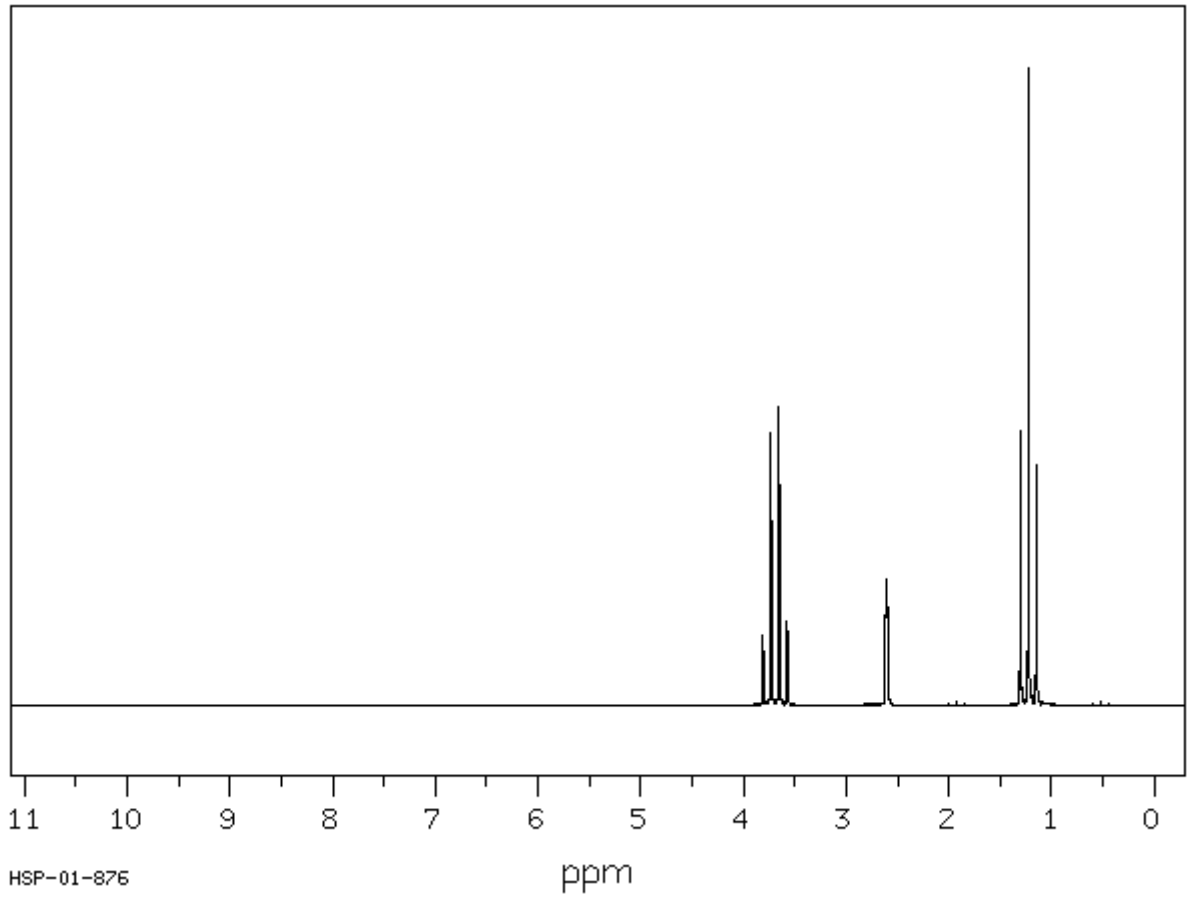
   b) The standard for comparison which gives a peak at 0 (often left out when these spectra are drawn) is tetramethylsilane (TMS). Draw its structure, and explain briefly why it is chosen as the standard.

2. a) The ^1H NMR spectrum for methoxymethane, CH_3-O-CH_3, is shown below. Explain why there is only one peak in the spectrum.



b) The horizontal scale on these spectra is in terms of "ppm" - parts per million. Explain what that means by considering the peak in the spectrum above.

c) The ^1H NMR spectrum for ethanol, the isomer of methoxymethane, is:



This consists of 3 clusters of peaks (actually one of the "clusters" only contains a single peak!). Thinking about the clusters as a whole, and not as individual sub-peaks, the areas under the three clusters are in the ratio 2 : 1 : 3. Account for this spectrum as fully as you can.

(At them moment you can't say anything about the individual sub-peaks. That will come in a later page about high resolution NMR. Unfortunately I can't find a reliable source of data about low resolution NMR where this problem would be conveniently hidden!)

d) How many peaks (counting clusters of peaks as above) would you expect to find in the H-1 NMR spectrum for

(i) pentan-3-one, $CH_3CH_2COCH_2CH_3$

(ii) pentan-2-one, $CH_3CH_2CH_2COCH_3$?

The spectra in this file are taken from the SDBS (SDBSWeb : http://sdbs.db.aist.go.jp (National Institute of Advanced Industrial Science and Technology, 24/8/2014).